

Mechanistic Study of Styrene Aziridination by Iron(IV) Nitrides

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General Procedures

All air-sensitive materials were handled under a nitrogen atmosphere by standard Schlenk techniques or in an M. Braun Labmaster glovebox unless otherwise noted. Prior to use glassware was dried at 150 °C overnight. Deuterated benzene was degassed and dried over molecular sieves (3 Å) in a storage flask filled with nitrogen. The dryness was periodically tested with a drop of Na/benzophenone in a tetrahydrofuran solution. The compounds $\text{PhB}(\text{tBuIm})_3\text{Fe}\equiv\text{N}$ ¹ and 4-chloro- β -deutero styrene² were prepared according to literature procedures, while 4-dimethylamino- β -deutero styrene was prepared from the appropriate aldehyde using a modified literature procedure.¹ ¹H NMR data were recorded on a Varian Unity 400 spectrometer (400 MHz) at 22 °C.

Reaction Monitoring

To a J-Young tube, was added $\text{PhB}(\text{tBuIm})_3\text{Fe}\equiv\text{N}$ (10 mg, 0.016 mmol, 1 equiv) and ca. 1 equiv. of the corresponding styrene as 0.3 mL of a C_6D_6 solution (1.5 mL total volume, containing 5 equivalents of styrene). The ¹H NMR spectrum of the reaction mixture was promptly obtained after addition of styrene, allowing the exact quantity of styrene to be determined by the integration of styrene and $\text{PhB}(\text{tBuIm})_3\text{Fe}\equiv\text{N}$ resonances. The tube was heated to 65 °C and the ¹H NMR spectrum of the reaction mixture was collected at regular time intervals with a thirty second relaxation delay. Reaction plots were generated from the integrated spectra, where were normalized to residual tetrahydrofuran present in the solution. The average of two resonances for each species was used to determine the molar concentration with an estimated error of less than 5 %.

¹ Scepaniak, J. J.; Fulton, M. D.; Bontchev, R. P.; Duesler, E. N.; Kirk, M. L.; Smith, J. M. *J. Am. Chem. Soc.* **2008**, *130*, 10515-10517.

² Robiette, R.; Pospíšil, J. *Eur. J. Org. Chem.*, **2013**, 836-840.

Table S1. Selected bond distances (Å) and angles (°) in **1**. X-ray crystal structure with atom labeling scheme shown for reference.

Parameter	1 ($S = 0$)	1 ($S = 1$)	1 (Crystal)
Fe–N (Å)	1.498	1.558	1.512(1)
Fe–C1 (Å)	1.936	1.982	1.915(1)
Fe–C2 (Å)	1.965	2.153	1.928(1)
Fe–C3 (Å)	1.964	2.018	1.928(1)
C1–Fe–C2 (°)	95.873	89.248	96.35(5)
C1–Fe–C3 (°)	95.864	92.806	97.90(5)
C2–Fe–C3 (°)	93.731	88.571	94.44(5)
B–Fe–N (°)	179.220	156.091	178.56(5)

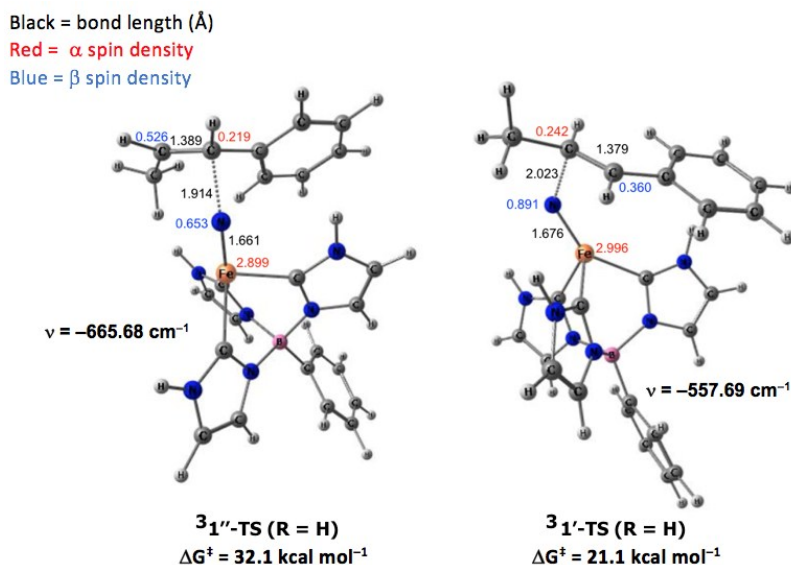
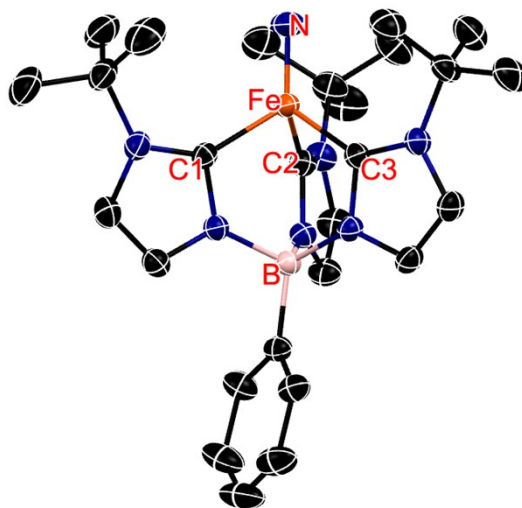


Figure S1. Comparison of formation of C–N bond through β and α carbons of (*Z*)-prop-1-en-1-ylbenzene during addition to **1**, using a small model where R groups on the NHC donors are truncated from ^tBu to H.

The barrier to the initial C–N bond formation is 21.1 kcal mol⁻¹ when the β carbon is attacked, but 32.1 kcal mol⁻¹ when bond formation proceeds through the α carbon. This TS, ³1''-TS, leads to a large accumulation of spin density (0.526 β) on the α carbon, which is unable to be stabilized by the phenyl moiety as in ³1'-TS.

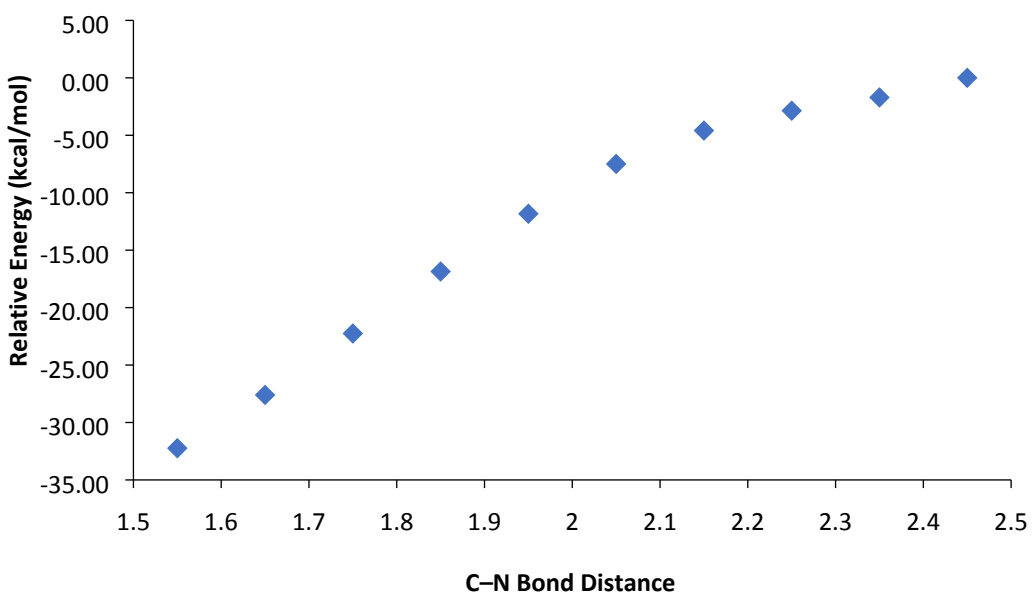


Figure S2. Linear Synchronous transit of electronic potential energy surface for ring closure on the $S = 2$ potential energy surface.

A scan of the potential energy surface for the quintet state shows that as the carbon-nitrogen distance is frozen at various distances along the bond formation coordinate while the rest of the molecule is optimized that the electronic potential energy continuously decreases as the bond is shortened. This suggests that this process has no barrier on the electronic potential energy surface and we were unable to optimize a transition state for C–N bond formation on the $S = 2$ surface.

Table S2. Mulliken spin densities on important atoms for selected structures.

	Fe	N	C1	C2
⁵ 1 (R = ^t Bu)	3.135 α	0.654 α	---	---
³ 1 (R = ^t Bu)	1.809 α	0.169 α	---	---
¹ 1 (R = ^t Bu)	0.000	0.000	---	---
⁵ 1-TS (R = ^t Bu)	3.463 α	0.480 α	0.161 α	0.281 β
³ 1-TS (R = ^t Bu)	2.626 α	0.488 β	0.145 α	0.258 β
¹ 1-TS (R = ^t Bu) (CSS)	0.000	0.000	0.000	0.000
¹ 1-TS (R = ^t Bu) (OSS)	0.617 β	0.268 α	0.162 β	0.379 α
⁵ 1a (R = ^t Bu)	3.325 α	0.422 β	0.004 β	0.772 α
³ 1a (R = ^t Bu)	3.208 α	0.416 β	0.086 α	0.671 β
¹ 1a (R = ^t Bu)	1.335 β	0.375 α	0.110 β	0.743 α
³ 1a-TS (R = ^t Bu)	1.847 α	0.428 β	0.021 α	0.478 α
¹ 1a-TS (R = ^t Bu)	0.000	0.000	0.000	0.000
⁵ 2 (R = ^t Bu)	3.685 α	0.115 α	0.011 α	0.013 α
³ 2 (R = ^t Bu)	2.092 α	0.071 β	0.020 α	0.016 α
¹ 2 (R = ^t Bu)	0.000	0.000	0.000	0.000
³ 1-TS (<i>p</i> -NO ₂)	1.781 α	0.044 β	0.060 β	0.182 α
³ 1-TS (<i>p</i> -H)	2.626 α	0.488 β	0.145 α	0.258 β
³ 1-TS (<i>p</i> -NMe ₂)	2.715 α	0.523 β	0.172 α	0.321 β

Table S3. Computed energy components of the optimized structures in eV.

	E(SCF) /TZ /eV cc-pvtz(-f)	ZPE	-TS (338.15 K)	G(solv) ($\epsilon=2.284$)	G(sol)
⁵ 1 (R = ^t Bu)	-43100.025	16.984	3.499	-0.281	-43086.822
³ 1 (R = ^t Bu)	-43100.844	17.019	3.454	-0.255	-43087.534
¹ 1 (R = ^t Bu)	-43101.130	17.050	3.356	-0.212	-43087.648
Styrene	-8428.929	3.633	-1.270	-0.071	-8426.637
(Z)-prop-1-en-1-ylbenzene	-9499.176	4.410	-1.366	-0.065	-9496.197
(p-NO ₂ C ₆ H ₄)CH=CH ₂	-13995.698	3.708	-1.480	-0.163	-13993.634
(p-NMe ₂ C ₆ H ₄)CH=CH ₂	-12075.774	5.624	-1.596	-0.105	-12071.850
⁵ 1-TS (R = ^t Bu)	-51529.082	20.620	-4.137	-0.219	-51512.818
³ 1-TS (R = ^t Bu)	-51529.578	20.648	-4.073	-0.214	-51513.217
¹ 1-TS (CSS) (R = ^t Bu)	-51529.637	20.707	-3.777	-0.213	-51512.920
¹ 1-TS (OSS) (R = ^t Bu)	-51529.696	20.684	-3.871	-0.212	-51513.094
⁵ 1a (R = ^t Bu)	-51530.079	20.618	-4.151	-0.225	-51513.837
³ 1a (R = ^t Bu)	-51530.300	20.715	-4.109	-0.214	-51513.908
¹ 1a (R = ^t Bu)	-51530.309	20.691	-3.907	-0.206	-51513.731
³ 1a-TS (R = ^t Bu)	-51530.239	20.683	-3.994	-0.206	-51513.756
¹ 1a-TS (R = ^t Bu)	-51529.883	20.707	-3.900	-0.203	-51513.279
⁵ 2 (R = ^t Bu)	-51531.611	20.692	-4.016	-0.218	-51515.153
³ 2 (R = ^t Bu)	-51531.039	20.720	-3.909	-0.210	-51514.437
¹ 2 (R = ^t Bu)	-51530.849	20.761	-3.907	-0.203	-51514.197
⁵ 1 (R = H)	-30256.944	7.821	2.335	-0.595	-30252.053
³ 1 (R = H)	-30257.867	7.851	2.317	-0.544	-30252.877
¹ 1 (R = H)	-30258.103	7.871	2.215	-0.484	-30252.932
⁵ 1a (R = H)	-38686.852	11.479	-2.994	-0.431	-38678.798
³ 1a (R = H)	-38687.559	11.548	-2.899	-0.412	-38679.322
¹ 1a (R = H)	-38687.229	11.552	-2.862	-0.431	-38678.971
⁵ 1-TS (R = H)	-38686.057	11.452	-3.025	-0.454	-38678.085
³ 1-TS (R = H)	-38686.797	11.510	-2.913	-0.409	-38678.609
¹ 1-TS (CSS) (R = H)	-38686.627	11.514	-2.864	-0.404	-38678.381
¹ 1-TS (OSS) (R = H)	-38686.373	11.486	-2.900	-0.416	-38678.203
³ 1a-TS (R = H)	-38687.313	11.502	-2.902	-0.367	-38679.080
¹ 1a-TS (R = H)	-38687.194	11.521	-2.727	-0.374	-38678.774
⁵ 2 (R = H)	-38688.473	11.527	-3.009	-0.375	-38680.330
³ 2 (R = H)	-38688.141	11.557	-2.915	-0.369	-38679.868
¹ 2 (R = H)	-38688.232	11.582	-2.821	-0.347	-38679.819
³ 1'-TS (R = H)	-39756.910	12.145	-2.502	-0.416	-39747.683
³ 1'-TS (R = H)	-39757.368	12.135	-2.542	-0.386	-39748.161
⁵ 1a (p-NO ₂)	-44254.142	11.567	-3.197	-0.530	-44246.303
³ 1a (p-NO ₂)	-44254.393	11.625	-3.096	-0.517	-44246.380
¹ 1a (p-NO ₂)	-44254.456	11.633	-3.085	-0.523	-44246.431
⁵ 1a (p-NMe ₂)	-42333.810	13.465	-3.249	-0.472	-42324.066
³ 1a (p-NMe ₂)	-42334.351	13.530	-3.227	-0.469	-42324.518
¹ 1a (p-NMe ₂)	-42333.986	13.536	-3.166	-0.460	-42324.076
⁵ 1-TS (p-NO ₂)	-44253.036	11.546	-3.145	-0.492	-44245.128
³ 1-TS (p-NO ₂)	-44253.773	11.598	-3.112	-0.529	-44245.817
¹ 1-TS (CSS) (p-NO ₂)	-44253.505	11.580	-2.966	-0.516	-44245.407

¹¹Ts (OSS) (<i>p</i>-NO₂)	-44253.514	11.556	-3.105	-0.528	-44245.591
⁵¹Ts (<i>p</i>-NMe₂)	-42332.848	13.440	-3.347	-0.503	-42323.257
³¹Ts (<i>p</i>-NMe₂)	-42333.555	13.490	-3.255	-0.451	-42323.770
¹¹Ts (CSS) (<i>p</i>-NMe₂)	-42333.496	13.498	-3.180	-0.433	-42323.612
¹¹Ts (OSS) (<i>p</i>-NMe₂)	-42333.536	13.475	-3.201	-0.444	-42323.707
^{31a}Ts (<i>p</i>-NO₂)	-44254.302	11.597	-3.080	-0.499	-44246.284
^{11a}Ts (<i>p</i>-NO₂)	-44254.005	11.623	-3.004	-0.493	-44245.879
^{31a}Ts (<i>p</i>-NMe₂)	-42334.118	13.494	-3.204	-0.400	-42324.228
^{11a}Ts (<i>p</i>-NMe₂)	-42334.006	13.507	-3.166	-0.414	-42324.079
⁵² (<i>p</i>-NO₂)	-44255.325	11.603	-3.203	-0.471	-44247.396
⁵² (<i>p</i>-NMe₂)	-42333.108	13.494	-3.268	-0.400	-42323.282

Table S4. Cartesian Coordinates of all optimized structures.

⁵¹(R=ⁿBu)

Fe	17.158978322	3.920329140	10.004133620
B	18.935139900	6.421812989	10.566379807
C	19.652965164	6.635603477	8.015883783
H	20.406530623	7.382910712	8.195715643
C	19.302024671	6.026349967	6.854997430
H	19.675922204	6.178965362	5.857856505
C	18.043995327	5.144263093	8.504877443
C	17.643750173	4.213942146	6.167202059
C	18.314035323	2.831460087	6.249112696
H	19.390327444	2.913734928	6.060885891
H	17.884799778	2.165105939	5.493222409
H	18.147809114	2.394427374	7.237736692
C	16.143487066	4.110947824	6.486039886
H	15.986915703	3.617856864	7.447977457
H	15.652846551	3.512843260	5.711019680
H	15.679918274	5.103223086	6.500880547
C	17.818026608	4.808413180	4.758145329
H	17.444559822	5.836340096	4.703841656
H	17.245568504	4.203075991	4.050465251
H	18.860121130	4.794386371	4.423691601
C	20.863902599	4.954356481	11.657475522
H	21.573803458	5.761866482	11.709159269
C	21.015059174	3.649669817	12.000038320
H	21.863305062	3.144602823	12.427590021
C	18.933877754	3.909735213	11.173456189
C	19.560388412	1.555110088	11.916570600
C	19.758148110	0.830892867	10.573491729
H	19.020434541	1.183207912	9.847048453
H	19.628856525	-0.247976797	10.711063834
H	20.767721782	1.007685166	10.185991827
C	20.550507181	1.014715530	12.963684706
H	21.584167689	1.018768907	12.603746566
H	20.291477490	-0.023900376	13.185286991
C	20.500787028	1.582446537	13.898667021
C	18.126279152	1.359534074	12.434424569
H	17.962963890	1.933540895	13.352801726
H	17.967353578	0.299284730	12.657631833
H	17.398672143	1.661520281	11.677843706
C	16.955307649	7.679026332	11.797934197
H	17.542873775	8.557015258	12.005770357
C	15.659256800	7.411651248	12.101252008
H	14.932513430	8.014696820	12.616866506
C	16.501628134	5.626744628	11.008879009
C	14.090466064	5.411799021	11.702583718
C	14.311643962	4.103153317	12.482515768
H	15.020325242	3.450380144	11.966304801
H	13.364332272	3.564356554	12.586181225
H	14.702636781	4.313042717	13.483309027
C	13.583274178	5.121875639	10.278540078
H	13.452554986	6.053765425	9.719180689
H	12.619187135	4.605219491	10.321977662
H	14.285639106	4.487568568	9.731600694
C	13.063708960	6.281568682	12.444328266
H	13.384923540	6.509657495	13.465568122
H	12.119006217	5.734920035	12.507801627
H	12.868376977	7.221082294	11.917598416
C	19.736635790	7.789787196	10.932575585
C	19.678823928	8.929615559	10.104802519
H	19.141079222	8.882628340	9.162877375
C	20.269460898	10.143803379	10.462181363
H	20.205979923	10.993564561	9.786974349
C	20.928349873	10.270412931	11.684778730
H	21.393215098	11.211697162	11.966076342
C	20.961684821	9.178020166	12.550902949

H	21.443560939	9.266649024	13.521489860
C	20.367311598	7.969537139	12.180596946
H	20.380178556	7.154799233	12.898170905
N	17.040405252	2.410676179	9.346512595
N	18.850795999	6.118082518	9.018284467
N	18.296249236	5.120270173	7.165524218
N	19.572201137	5.115850941	11.187087284
N	19.812517259	3.017549693	11.711890596
N	17.465450912	6.577533003	11.127927546
N	15.391575375	6.138463352	11.608051452

³¹(R=ⁿBu)

Fe	17.173130513	3.944773440	10.036985492
B	18.934108257	6.472061619	10.557122356
C	19.644982439	6.715442392	7.981459734
H	20.365298900	7.501527259	8.131102783
C	19.315057574	6.052601221	6.842780547
H	19.674506613	6.188144922	5.837841393
C	18.098543664	5.179016621	8.535592124
C	17.713019346	4.138397565	6.261856854
C	18.201054409	2.723459898	6.618859418
H	19.292252642	2.664150580	6.550944664
H	17.771795417	1.991203170	5.927447579
H	17.898993915	2.455912120	7.634486732
C	16.184916616	4.243025845	6.407192757
H	15.870407812	3.989392592	7.421993563
H	15.697861060	3.551206797	5.712423142
H	15.844766557	5.258695067	6.180059520
C	18.109657888	4.472419319	4.815270250
H	17.811801490	5.488409871	4.537608326
H	17.600119641	3.778340079	4.141763989
H	19.185524839	4.361770819	4.647064079
C	20.828626261	4.976442198	11.652147870
H	21.523989934	5.788517437	11.777116110
C	20.985512477	3.656219568	11.910752853
H	21.825791056	3.136804336	12.333678435
C	18.920704084	3.949222733	11.045635570
C	19.563163302	1.550490626	11.685758494
C	19.290038957	0.947004905	10.297443823
H	18.378875894	1.362152211	9.865054232
H	19.166982022	-0.137197961	10.386852947
H	20.130679977	1.142698383	9.622881556
C	20.816364247	0.880069619	12.276826278
H	21.692375218	0.996549523	11.630623230
H	20.619401163	-0.190855230	12.373656723
H	21.057047832	1.260932723	13.274294051
C	18.379220124	1.328516642	12.641900082
H	18.590332071	1.778772793	13.618041398
H	18.221774735	0.254505793	12.786301239
H	17.464496150	1.763087350	12.235221950
C	16.892532232	7.663971505	11.715435890
H	17.447652612	8.563110748	11.921706825
C	15.600660845	7.357730627	11.981633422
H	14.842085560	7.944509351	12.466650852
C	16.530158106	5.582467414	10.949686100
C	14.066514071	5.349127212	11.592967896
C	14.222317633	4.146443475	12.539057973
H	14.957608230	3.439426545	12.150339207
H	13.261364094	3.631442818	12.641865910
H	14.538601033	4.484181107	13.532073709
C	13.639481126	4.907034009	10.182660682
H	13.556421116	5.774081411	9.518203561
H	12.662084368	4.416617957	10.232586250
H	14.357010184	4.202306932	9.760382888
C	12.996385312	6.300060471	12.156691514
H	13.224124511	6.620199380	13.178261961
H	12.042741655	5.766418128	12.187351172
H	12.861316970	7.186302087	11.528422601
C	19.717801662	7.837108415	10.960317000

C	19.685182114	8.982893933	10.139376449	H	12.656262145	4.495697208	10.252870488
H	19.162258884	8.948013562	9.188857397	H	14.330199565	4.409177272	9.666543908
C	20.281381298	10.188814406	10.515503822	C	13.075289502	6.157588671	12.386125060
H	20.238555513	11.043906290	9.845484771	H	13.385176313	6.381671092	13.412264642
C	20.920685844	10.299327072	11.749732980	H	12.137694317	5.597066400	12.439291895
H	21.391043731	11.233418052	12.045283396	H	12.868438675	7.098246366	11.864988139
C	20.928274926	9.200693125	12.608999764	C	19.734175695	7.840706504	10.954250408
H	21.394974480	9.278827952	13.587795295	C	19.700780743	8.978675311	10.123213378
C	20.328549997	8.000760380	12.220367135	H	19.171288310	8.938355184	9.175969119
H	20.323995298	7.178629096	12.929887942	C	20.304015237	10.185848816	10.484560999
N	16.333546834	2.689748640	10.421886062	H	20.261274457	11.034377945	9.805371294
N	18.872937976	6.193656742	9.004741120	C	20.949486205	10.307385256	11.714710523
N	18.350500773	5.114719924	7.195132553	H	21.425889724	11.242861859	11.998156644
N	19.552214007	5.154415454	11.150408885	C	20.953513292	9.218328061	12.586340552
N	19.801150009	3.025291994	11.540955109	H	21.422265757	9.304859477	13.564136674
N	17.457701347	6.570287677	11.080988927	C	20.346934614	8.017301283	12.212254155
N	15.378797366	6.068883943	11.500358407	H	20.336178992	7.205705107	12.933864570

11 (R=Bu)							

Fe	17.280038889	4.063459693	10.029126104				
B	18.950777870	6.470230281	10.578265387				
C	19.592897973	6.685853854	7.991797107				
H	20.302215355	7.484497152	8.126628698				
C	19.254808004	6.014133837	6.866089642				
H	19.591794235	6.153939042	5.854545117				
C	18.105693684	5.104263000	8.581630831				
C	17.691312570	4.073102732	6.286473171				
C	18.192348553	2.656523810	6.615774060				
H	19.283922317	2.608562509	6.532557459				
H	17.761679531	1.936625204	5.911475612				
H	17.901921277	2.369369390	7.627575306				
C	16.162370897	4.173682681	6.421807002				
H	15.842748018	3.923918537	7.434778532				
H	15.683502207	3.478704903	5.723866552				
H	15.824355193	5.188719566	6.184699557				
C	18.089703801	4.427488290	4.843697112				
H	17.778833120	5.441082502	4.569718029				
H	17.588321154	3.731746638	4.165130438				
H	19.167284695	4.329425383	4.675281334				
C	20.839351287	4.965286223	11.729881272				
H	21.542692337	5.768832997	11.867426747				
C	20.970686606	3.646956789	12.008288163				
H	21.791714100	3.117047361	12.457343067				
C	18.941175312	3.953602876	11.071115499				
C	19.516970282	1.559194428	11.732494306				
C	19.439055774	0.948278386	10.323106989				
H	18.618902400	1.390217512	9.755167830				
H	19.271719466	-0.131810023	10.394800118				
H	20.376847749	1.116206664	9.781721191				
C	20.661413473	0.888569235	12.511274851				
H	21.618820683	0.960408220	11.984535295				
H	20.428657846	-0.174199275	12.622176449				
C	20.776671029	1.310205188	13.515300432				
C	18.201714284	1.359861211	12.505178776				
H	18.275163259	1.804392418	13.504055464				
H	17.998145773	0.289649059	12.617833441				
H	17.364669006	1.818854304	11.976706118				
C	16.913271885	7.651175635	11.787504796				
H	17.468244739	8.547240561	12.010372408				
C	15.628857873	7.329194451	12.066807748				
H	14.872179249	7.896478311	12.578586819				
C	16.552076084	5.585855640	10.977404968				
C	14.114545230	5.301368059	11.643792065				
C	14.340889049	3.993724341	12.422741018				
H	15.068330509	3.358720159	11.913967084				
H	13.397289820	3.444090091	12.507610115				
H	14.706252382	4.210260668	13.432929117				
C	13.614791749	5.024388512	10.215345046				
H	13.468766551	5.965418604	9.673166234				

Styrene							

C	0.795268545	-0.458122837	-1.817887934				
C	-0.445483678	-0.953189102	-1.405610226				
C	1.716679544	0.002738295	-0.882972851				
H	-1.161116774	-1.314145499	-2.138569974				
H	2.678994849	0.372803840	-1.223488699				
C	-0.753072209	-0.984687249	-0.045659532				
C	1.420540706	-0.014571846	0.492050833				
H	-1.712199883	-1.370169574	0.288681666				
C	0.171768389	-0.522293318	0.889332625				
H	-0.074793812	-0.549479196	1.948214924				
H	1.046589050	-0.436233298	-2.874659404				
C	2.354493993	0.466490304	1.524013777				
C	3.518663370	1.099218311	1.335279947				
H	2.030603158	0.289242251	2.548278185				
H	4.129075787	1.401205331	2.180439044				
H	3.913858576	1.327115801	0.350756990				

(Z)-prop-1-en-1-ylbenzene							

C	0.635860621	-0.242812526	-1.831221207				
C	-0.341145180	-1.127380578	-1.372286805				
C	1.477683940	0.410243790	-0.931299003				
H	-0.996835401	-1.632545492	-2.075713078				
H	2.2011151058	1.127277353	-1.303459589				
C	-0.480395409	-1.343597328	0.000386503				
C	1.365505993	0.188113925	0.453586256				
H	-1.245978864	-2.019760034	0.371118845				
C	0.356365234	-0.686692182	0.898578557				
H	0.240191690	-0.856757106	1.966218487				
H	0.735881517	-0.049203210	-2.895750775				
C	2.215966056	0.851187893	1.459261796				
C	3.508482338	1.211074505	1.377265523				
H	1.719980807	1.029157608	2.413212846				
H	3.931469960	1.696696724	2.256415182				
C	4.470287967	1.001931598	0.242897627				
H	5.443367080	0.676286783	0.629016536				
H	4.118307182	0.253093562	-0.469838033				
H	4.652090734	1.934271198	-0.308809920				

(p-NO₂C₆H₄)CH=CH₂							

C	0.709110656	-0.347177253	-1.831829114				
C	-0.469946255	-0.944924324	-1.382882651				

C	1.633182398	0.102347429	-0.899202403	C	20.789883954	8.743415397	13.086736147
H	2.553206884	0.557867994	-1.249409148	H	21.326371160	8.643065789	14.027152121
C	-0.737804107	-1.104780891	-0.026070715	C	20.307788342	7.603448597	12.439647724
C	1.396779720	-0.035587275	0.483519000	H	20.460152098	6.641679336	12.920750692
H	-1.661861001	-1.577374191	0.282511718	N	16.069912804	3.034783662	8.715593832
C	0.198664695	-0.649890710	0.894555714	N	18.782908483	6.451750550	8.969729535
H	0.001170706	-0.768977634	1.956134050	N	18.289842513	5.849334490	6.941348525
H	0.880838517	-0.249403492	-2.896469299	N	19.780074735	5.023887041	10.751396571
C	2.342199022	0.425844570	1.511849139	N	20.323531657	2.923980956	10.622056899
C	3.471935371	1.118739409	1.320810081	N	17.512086923	6.156506413	11.190878577
H	2.062703662	0.168361669	2.532488575	N	15.561526012	5.346882331	11.726998500
H	4.094372945	1.407149882	2.161215438	C	15.149285193	1.456240558	7.661691209
H	3.817222965	1.426959039	0.338642042	C	16.056137978	0.430887077	7.666828685
N	-1.447445894	-1.427415470	-2.365359762	C	16.230961938	-0.561588276	8.716596383
O	-2.475894736	-1.953777525	-1.939085130	C	15.514071475	-0.536370413	9.933424178
O	-1.181975602	-1.276705611	-3.558320994	C	17.161602048	-1.607412404	8.534234511

(p-NMe₂C₆H₄)CH=CH₂

C	0.2836982317	0.0570725479	-1.6444488976	C	14.809348566	0.267576868	10.121223624
C	-0.5664284431	-1.0235873599	-1.3074171306	H	17.727492701	-1.648638549	7.605807294
C	1.2598904744	0.5060501011	-0.7680555327	H	15.152590858	-1.464024197	11.834864124
H	1.8850087207	1.3388024546	-1.0771503147	H	18.084318941	-3.376636119	9.334956982
C	-0.3892089385	-1.6021331603	-0.0313690681	H	16.794395793	-3.299681291	11.466440380
C	1.4496220546	-0.0753139046	0.4980446595	H	14.308453843	1.471897703	8.344551734
H	-1.0216871080	-2.4177178377	0.2962847288	H	16.772529560	0.377146339	6.848167724
C	0.5946960059	-1.1376595385	0.8330596487	C	14.346933913	4.471338494	11.771577542
C	0.6983062284	-1.6129469352	1.8062001125	C	13.598583794	4.598583657	10.433423299
H	0.1814360339	0.5570889022	-2.5995312571	H	14.225526037	4.243299136	9.610816813
C	2.4658496425	0.3716775743	1.4578617353	H	12.684135150	3.995792535	10.463723844
C	3.3577677872	1.3617565324	1.3130509792	H	13.314827908	5.640905991	10.250453019
H	2.4740673705	-0.1854477727	2.3955113224	C	13.432725107	4.919942646	12.923162716
H	4.0650281309	1.5944899698	2.1023851313	H	13.049307477	5.934831706	12.775684021
H	3.4246765277	1.9661754235	0.4129347129	H	12.570720288	4.248519602	12.964226874
N	-1.5252077883	-1.5006244478	-2.1968370705	H	13.940497191	4.870218823	13.892044772
C	-2.5479450333	-2.4070006444	-1.7018563871	C	14.794270852	3.019743592	12.015766284
H	-3.1993089219	-2.6988808673	-2.5279699863	H	13.912627872	2.377723525	12.119844158
H	-2.0978860091	-3.3222629711	-1.3033944189	H	15.389872707	2.653709353	11.176154608
H	-3.1710752730	-1.9608800477	-0.9099463770	H	15.382471023	2.945140276	12.936908515
C	-1.8586331116	-0.7040430728	-3.3658863910	C	17.681684540	5.120277293	5.785888260
H	-2.5860776271	-1.2457254083	-3.9735883609	C	16.150481301	5.168064815	5.928084384
H	-2.2838242989	0.2800720394	-3.1103422709	H	15.685765085	4.671001466	5.069348482
H	-0.9745083226	-0.5398156828	-3.9898132796	H	15.835728734	4.658475329	6.842798940

⁵¹Ts (R='Bu)

Fe	17.358294777	3.846431107	9.448393699	H	17.827429504	3.144103554	6.689356110
B	18.941872138	6.349490181	10.534480782	H	17.807060105	3.135591245	4.915919946
C	19.482828777	7.284465460	8.110864074	H	19.279359178	3.633242481	5.773755425
H	20.149341214	8.056508425	8.456031431	C	18.101832812	5.796440826	4.471036132
C	19.168247305	6.921270826	6.841547407	H	19.184943313	5.756561073	4.314014161
H	19.492094194	7.341730552	5.905826639	H	17.629290654	5.266869517	3.639335820
C	18.069196189	5.538576816	8.250269131	H	17.776472110	6.840885031	4.426596267
C	21.115876418	4.920729761	11.101963752	C	20.223766793	1.447589078	10.407471732
H	21.721278920	5.773151743	11.359122022	C	19.944505327	1.183547403	8.917521199
C	21.458680250	3.608278915	11.037344220	H	20.734756153	1.616607862	8.294629086
H	22.397024245	3.129331353	11.255909806	H	19.902157539	0.105808336	8.731988748
C	19.294177612	3.794049934	10.418241759	H	18.985159932	1.611148034	8.613836142
C	16.968298878	6.987870029	12.158197900	C	19.087184643	0.897453224	11.286439040
H	17.479081850	7.858427525	12.532153326	H	18.128592140	1.345910266	11.017006302
C	15.753406646	6.487353537	12.496010478	H	18.999123295	-0.184939990	11.153357760
H	15.036385221	6.847796955	13.212176488	H	19.284237811	1.106730749	12.343632309
C	16.638243484	5.145677021	10.919437972	C	21.547618206	0.776158671	10.806238083
C	19.611476606	7.668294669	11.215189027	H	21.793622873	0.953067489	11.858387861
C	19.370545535	8.964163170	10.714553630	H	21.449052542	-0.303543045	10.665754709
H	18.774559962	9.089598369	9.815358892	H	22.383926072	1.115205044	10.186059025
C	19.846492244	10.112383246	11.351720418	H	15.034967559	2.066919533	6.774726589
H	19.639622097	11.090696785	10.924677460	*****			
C	20.572828483	10.006664038	12.537302239	³¹Ts (R='Bu)			
H	20.947959405	10.896720750	13.035753550	*****			

³¹Ts (R='Bu)

Fe	17.651662713	3.390946793	8.897749896
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B 18.546458370 6.109671416 10.232436137
 C 19.317519724 7.178434467 7.911508305
 H 19.753201350 8.063408449 8.342273090
 C 19.281033316 6.776499013 6.615059086
 H 19.650324915 7.265599494 5.730673956
 C 18.286192881 5.180761526 7.867063451
 C 20.756463256 5.039422805 11.220330648
 H 21.153244189 5.972753497 11.581418599
 C 21.311862650 3.804205376 11.231598653
 H 22.255602926 3.479726411 11.631895578
 C 19.302066891 3.649908241 10.203008240
 C 16.170197840 6.362342933 11.341803851
 H 16.425389099 7.286428805 11.831847028
 C 15.002775787 5.675398326 11.337951081
 H 14.071185068 5.898196140 11.826511966
 C 16.479426071 4.539438336 10.067499671
 C 18.832035748 7.501331606 11.022740083
 C 18.489279415 8.754538557 10.475432847
 H 18.067967011 8.807493035 9.476017435
 C 18.642776241 9.947335513 11.185940908
 H 18.372623130 10.891705707 10.719422348
 C 19.130392632 9.927602839 12.492325446
 H 19.256676721 10.853192424 13.048177066
 C 19.431595097 8.700827730 13.083431192
 H 19.782792509 8.663261037 14.111862753
 C 19.273474777 7.515661390 12.361521550
 H 19.482855286 6.577825420 12.867716446
 N 17.330661434 1.798430742 8.726065397
 N 18.678152315 6.210885844 8.665473820
 N 18.629907495 5.549152349 6.599305097
 N 19.512940325 4.932228642 10.619630292
 N 20.405611760 2.950055746 10.609710665
 N 17.072699867 5.660223965 10.559080823
 N 15.199109283 4.550899795 10.539888870
 C 16.406536623 0.231651846 8.039987033
 C 16.042441405 0.528391458 6.738208889
 C 16.862066237 0.333158251 5.559534866
 C 18.173363120 -0.194838174 5.601964128
 C 16.347214056 0.675598376 4.287620540
 C 18.917600440 -0.370316654 4.440320381
 C 17.094079882 0.499565259 3.126791707
 C 18.388264428 -0.024673457 3.192415394
 H 18.615235957 -0.453641355 6.558818838
 H 15.340455584 1.083312626 4.224312844
 H 19.925097107 -0.774055221 4.507548107
 H 16.666124937 0.773614331 2.165273459
 H 18.975211330 -0.160370732 2.288300324
 H 17.219550415 -0.459578110 8.237775602
 H 15.094487203 1.038954873 6.578095126
 H 15.640108466 0.238507568 8.808351195
 C 20.632251651 1.482174657 10.418776885
 C 19.471127609 0.711912800 11.070688475
 C 21.950240806 1.068621828 11.096301098
 H 22.819460882 1.562263354 10.649538354
 H 21.940616248 1.272418856 12.171813173
 H 22.082421066 -0.008770822 10.965188954
 H 19.406406253 0.952359139 12.137528724
 H 19.643962857 -0.365262013 10.972138764
 H 18.523441262 0.959775370 10.588546712
 C 18.383223689 4.720402559 5.380468250
 C 16.907933173 4.287429930 5.372805277
 C 19.316985992 3.499543824 5.421244195
 H 20.364253740 3.820169318 5.453372277
 H 19.110891204 2.886950072 6.301640970
 H 19.168125483 2.876467387 4.534624791
 H 16.677324476 3.665285632 6.240783873
 H 16.701912589 3.698308233 4.474258458
 H 16.249850086 5.163340491 5.381302252
 C 14.158884148 3.513752527 10.259180991
 C 14.590525459 2.193679508 10.920926967

C 14.009131917 3.360629022 8.735297327
 H 13.727722099 4.316717624 8.280742546
 H 14.939982469 3.017356202 8.279987407
 H 13.224229474 2.629920271 8.513188572
 H 13.847224765 1.414526873 10.720128837
 H 14.669247524 2.319647547 12.006232877
 C 20.730995768 1.184331692 8.912543140
 H 21.547728750 1.758238069 8.460991188
 H 20.935493133 0.119322553 8.758383971
 H 19.798237752 1.435176695 8.405322383
 C 18.673323414 5.553740817 4.121750538
 H 19.729794016 5.830426684 4.043522580
 H 18.427635755 4.954068878 3.241445021
 H 18.066543572 6.464651831 4.088513284
 H 15.559353134 1.867531411 10.537140994
 C 12.809842239 3.960564825 10.847390749
 H 12.474921078 4.913376427 10.424856390
 H 12.057247085 3.205774982 10.603328536
 H 12.843196295 4.048939920 11.937947587

¹H-TS (CSS) (R=^tBu)

Fe 17.892446301 3.197356051 9.987185681
 B 18.523628798 6.162688073 10.375721725
 C 18.465978228 6.563338303 7.734716541
 H 18.794036694 7.587989897 7.774408722
 C 18.204671859 5.781770105 6.660397037
 H 18.235145036 6.020604856 5.612591031
 C 17.919640378 4.522860852 8.519375542
 C 21.040363806 5.577081958 11.030915972
 H 21.378763582 6.598151235 11.071473928
 C 21.738167468 4.428829566 11.193132165
 H 22.775604901 4.284443901 11.434577284
 C 19.604662726 3.873413685 10.697203184
 C 16.481793675 6.413560655 12.034190636
 H 16.654372565 7.461360223 12.214974033
 C 15.526778990 5.589789089 12.524882082
 H 14.722237007 5.797026054 13.207340015
 C 16.846708935 4.375072081 11.146173398
 C 18.735808753 7.745645998 10.675106713
 C 18.034380719 8.735427982 9.955829904
 H 17.370432143 8.442975880 9.147762079
 C 18.137347721 10.095476190 10.258790856
 H 17.583873676 10.822144844 9.668659812
 C 18.938538815 10.521009908 11.318631020
 H 19.027528685 11.578317687 11.554436599
 C 19.602263181 9.564166205 12.086715377
 H 20.204343858 9.871538228 12.938540491
 C 19.489884713 8.207093264 11.773360965
 H 19.990238782 7.492705963 12.420048715
 N 17.676918786 1.663641805 9.763880550
 N 18.254088636 5.800115125 8.869162139
 N 17.854871055 4.523638876 7.148958469
 N 19.726936920 5.233239282 10.763380659
 N 20.845498396 3.375600106 11.000307431
 N 17.283957214 5.663837970 11.190477081
 N 15.755159519 4.327706282 11.972571295
 C 16.878043580 0.142481947 9.297263608
 C 17.835963623 -0.850572688 9.502288977
 C 18.098721439 -1.538699873 10.741112955
 C 17.305265791 -1.381561516 11.900312075
 C 19.195374776 -2.426998727 10.823833750
 C 17.601454606 -2.065826547 13.070925432
 C 19.486017297 -3.113402461 11.0996163301
 C 18.692924787 -2.936277496 13.131124496
 H 16.458390836 -0.706258022 11.880509495
 H 19.819824121 -2.567000886 9.945866050
 H 16.979115657 -1.917287091 13.948307889
 H 20.336958071 -3.787208226 12.028398165
 H 18.922427503 -3.465580646 14.050233616

H	16.011715737	0.169426720	9.953078781	H	20.153604852	9.885338814	12.950996999
H	18.549359010	-1.027711570	8.701369725	C	19.467971553	8.215550816	11.775339405
H	16.631970387	0.375252172	8.266593977	H	19.975560098	7.504481947	12.419854956
C	17.462864076	3.368307123	6.286192957	N	17.641894084	1.689701040	9.764160164
C	16.073657972	2.880336645	6.731259262	N	18.260314219	5.804504842	8.865910589
C	18.521814853	2.259977382	6.4161133626	N	17.881258282	4.531143835	7.138134752
H	19.501912261	2.632190676	6.098405693	N	19.740155460	5.251572496	10.761773078
H	18.596279896	1.917020113	7.449646877	N	20.878498817	3.405950967	10.990885631
H	18.254247301	1.411115572	5.777159093	N	17.289156146	5.662507658	11.192127613
H	16.087357449	2.590517257	7.783368528	N	15.770410888	4.321092315	11.987211756
H	15.767089236	2.019245864	6.128049096	C	16.807262947	0.068714556	9.282974862
H	15.330068129	3.673884025	6.600650835	C	17.750667937	-0.928544147	9.503762182
C	14.928511881	3.118572456	12.254859176	C	18.010071423	-1.601957231	10.757368263
C	15.820889983	2.057010026	12.919386185	C	17.223862456	-1.414617911	11.917968459
C	14.338532939	2.606980177	10.929760834	C	19.101885602	-2.495773679	10.849617369
H	13.692776359	3.368218931	10.478942958	C	17.523412139	-2.078297588	13.101879680
H	15.136318413	2.367328465	10.223799434	C	19.397871573	-3.160194576	12.035200004
H	13.738861485	1.707688326	11.106638725	C	18.611691121	-2.954661591	13.172178849
H	16.643157568	1.773654058	12.259670678	H	16.379199275	-0.734740197	11.889257186
H	15.229503653	1.165116368	13.154110467	H	19.721229565	-2.656300152	9.969987674
H	16.241897057	2.443172833	13.853883146	H	16.906387666	-1.909695221	13.980954195
C	21.226950500	1.931107682	11.116024832	H	20.246818689	-3.837960300	12.075688888
C	21.133168713	1.276512895	9.727453109	H	18.843973071	-3.467692446	14.101095586
C	20.293280918	1.253041298	12.131344600	H	15.956716039	0.159669914	9.951637640
H	20.390238730	1.731190698	13.112595604	H	18.453678938	-1.141323664	8.700117493
H	19.254852170	1.315269183	11.807192577	H	16.587887799	0.335372620	8.254218473
H	20.557367450	0.196050364	12.232533782	C	17.507522673	3.373702591	6.269533846
H	20.112138230	1.325838083	9.348062787	C	16.114072508	2.878566186	6.692606176
H	21.430799855	0.224785096	9.793705298	C	18.568038376	2.269273026	6.418077624
H	21.803807497	1.781291413	9.022805593	H	19.553497926	2.645977395	6.123223341
C	17.382136543	3.815242019	4.816420376	H	18.620318536	1.921486058	7.451248489
H	18.353639220	4.138844461	4.429317355	H	18.317208964	1.422252340	5.769993267
H	17.056870596	2.963348460	4.212763960	H	16.114817024	2.582519121	7.742919418
H	16.656402208	4.621744557	4.671498431	H	15.820379982	2.019212473	6.080348412
C	13.778159805	3.479730219	13.209614798	H	15.368970892	3.669497829	6.554715589
H	13.112711325	4.237537293	12.783719612	C	14.954529056	3.107002760	12.282149377
H	13.182137302	2.581078992	13.392300727	C	15.863503941	2.049158522	12.930289653
H	14.144930699	3.834925550	14.177870713	C	14.343333625	2.594116137	10.967110228
C	22.675065819	1.815121920	11.623726022	H	13.683517990	3.351705448	10.530636239
H	22.808321301	2.292860001	12.599662779	H	15.128921705	2.360667594	10.246167116
H	22.912628020	0.754077615	11.739205586	H	13.752507287	1.690928144	11.154472540
H	23.399225013	2.237536146	10.919336382	H	16.670231875	1.762955442	12.253024335

¹H-TS (OSS) (R=^tBu)							

Fe	17.905934341	3.213018930	9.985671357	C	21.270170252	1.963686977	11.085814900
B	18.525770245	6.167938194	10.373541865	C	21.164368958	1.325892803	9.690171533
C	18.478984123	6.571720494	7.734981484	C	20.347669828	1.265552598	12.098061118
H	18.801550403	7.597843314	7.780274575	H	20.443404416	1.733383574	13.084302981
C	18.230080089	5.792176968	6.656144406	H	19.306690049	1.320973175	11.779013764
H	18.266224597	6.034622870	5.609267126	H	20.622968470	0.210075602	12.186996402
C	17.933954133	4.527501387	8.508013120	H	20.136416377	1.366424046	9.327343248
C	21.051173463	5.608557837	11.026481337	H	21.477350508	0.277460948	9.737053922
H	21.379328713	6.632857117	11.069422172	C	21.815970774	1.849045048	8.981179485
C	21.761791583	4.467185159	11.183947844	C	17.450968654	3.820549221	4.798659562
H	22.801293680	4.332648942	11.422879641	H	18.427492990	4.150215736	4.429759711
C	19.632765964	3.890831135	10.692564414	H	17.141951658	2.967016910	4.188787446
C	16.492219462	6.409007549	12.044324154	H	16.723133819	4.622778764	4.640508474
H	16.661783902	7.457349245	12.224182864	C	13.820076392	3.462507170	13.257750535
C	15.543916904	5.582058631	12.542625336	H	13.143563939	4.217338169	12.844239489
H	14.744294972	5.786693189	13.231582001	H	13.231520306	2.561013224	13.450306835
C	16.853555885	4.373330840	11.152445124	H	14.202487899	3.818829068	14.219576338
C	18.721990176	7.750418034	10.673557963	C	22.723286008	1.852570601	11.579504623
C	18.008390004	8.731772762	9.955691489	H	22.860510526	2.320854681	12.559517545
H	17.350204599	8.432046121	9.145601925	H	22.971752906	0.792626496	11.680996302
C	18.089793270	10.091052818	10.265996615	H	23.437299075	2.290197181	10.874024547
H	17.527089181	10.813281409	9.679181480	*****			
C	18.880818854	10.520791823	11.331339588	⁵1a (R=^tBu)			
H	18.952132101	11.578124568	11.573795409	*****			
C	19.558892846	9.572000991	12.096219518	Fe	17.720047855	3.744280107	9.776454537
				B	19.055082750	6.526687573	10.547712226

C	19.094429846	7.453158572	8.061493925	C	17.220403683	5.756778516	4.737843256
H	19.691194578	8.319578250	8.292037136	H	18.214645800	5.962951857	4.328707775
C	18.634503612	7.020408133	6.862291873	H	16.687393652	5.143278352	4.005806221
H	18.734967284	7.460628465	5.885040781	H	16.678687023	6.702596710	4.840138957
C	17.982543136	5.522255410	8.439911257	C	20.959884256	1.830052827	10.272789915
C	21.460554110	5.406261718	10.818345766	C	20.649392582	1.517777640	8.797936026
H	21.979045507	6.335848095	10.980606867	H	21.360727131	2.025566575	8.137766765
C	21.959422943	4.147988310	10.714848251	H	20.722294959	0.439775808	8.619328747
H	22.973597188	3.799474816	10.800599499	H	19.638654119	1.842852721	8.542110575
C	19.725393093	4.040521320	10.412653524	C	19.949611781	1.137512807	11.204754183
C	17.213801804	6.948191775	12.395951175	H	18.923727074	1.409386179	10.946328720
H	17.641058296	7.887721041	12.703329206	H	20.050075847	0.050809123	11.109459117
C	16.108070998	6.308749812	12.852659307	H	20.139325585	1.410458425	12.248357536
H	15.413535686	6.596738069	13.622314172	C	22.377781619	1.342345366	10.612656529
C	17.018938821	5.044012818	11.223472878	H	22.653107702	1.583199607	11.644486847
C	19.631333843	7.939558285	11.117345570	H	22.409665410	0.254784226	10.503126305
C	19.153590789	9.180558728	10.648853119	H	23.132160372	1.760537507	9.938374201
H	18.422054156	9.204376371	9.846616699	H	17.031757102	1.154121031	7.412544987
C	19.567879239	10.396939098	11.196756852	*****			
H	19.176811641	11.328973898	10.795573919	³1a (R=ⁱBu)			
C	20.470278690	10.417949069	12.260289415	*****			
H	20.799381594	11.361471706	12.687056764	Fe	17.849151585	3.686300042	9.211295501
C	20.923538056	9.206618626	12.783057145	B	18.925699990	6.362153803	10.541185661
H	21.601354376	9.199120316	13.633249211	C	19.153249087	7.639535288	8.211250012
C	20.500688555	7.997558825	12.225545594	H	19.671594083	8.490910487	8.618166802
H	20.844692063	7.076065786	12.686558886	C	18.828932149	7.364041285	6.922053312
N	16.989170459	2.249315709	9.156603019	H	18.990574166	7.946332480	6.031730308
N	18.661934662	6.552580335	9.026780019	C	18.136874122	5.633012240	8.200182707
N	17.939082390	5.838845990	7.110464559	C	21.338959136	5.306451175	10.923635107
N	20.087234833	5.328981679	10.661911633	H	21.798306822	6.229632270	11.233364970
N	20.876106388	3.309663321	10.476698706	C	21.894496741	4.080378854	10.756163644
N	17.769011386	6.166144559	11.394040684	H	22.904824421	3.751695879	10.925638353
N	15.998319487	5.122847519	12.122196190	C	19.707609267	3.938425037	10.196701645
C	16.361708170	1.327681208	8.284034949	C	16.857385853	6.441651997	12.172644124
C	15.984977431	-0.007968378	8.881958826	H	17.159372892	7.374724932	12.616911371
C	15.258589024	-1.023370793	8.213379189	C	15.780081804	5.664118074	12.438189388
C	14.797710588	-0.887167954	6.867968563	H	14.989372949	5.801842019	13.154418299
C	14.958691291	-2.250966861	8.876188071	C	16.969565375	4.662921476	10.801986501
C	14.091626150	-1.906207030	6.244819237	C	19.350597479	7.710285623	11.348755475
C	14.251013432	-3.260704623	8.243228573	C	18.845404975	8.979052648	10.998340989
C	13.809260664	-3.100832446	6.920508849	H	18.194373584	9.077442334	10.134722766
H	15.006479983	0.027798987	6.321489279	C	19.127786700	10.128294243	11.740800166
H	15.297275179	-2.383823920	9.901916560	H	18.720217755	11.085921675	11.425559306
H	13.754685937	-1.773465273	5.218843263	C	19.919629248	10.048390278	12.886560956
H	14.038982604	-4.184173800	8.776922516	H	20.146895424	10.940138060	13.464699852
H	13.256207292	-3.894424727	6.425544418	C	20.394344038	8.800655554	13.291096922
H	15.461804606	1.783479022	7.815809018	H	20.985912347	8.710997921	14.199192872
H	16.320689742	-0.188772325	9.902051809	C	20.102931319	7.659141478	12.539901668
C	14.916484279	4.107032823	12.275019045	H	20.458248912	6.701601927	12.909377945
C	14.125421909	4.026186390	10.956603386	N	17.328080800	2.355942899	8.203979166
H	14.777363756	3.729242850	10.131966466	N	18.697251981	6.590167330	8.991544187
H	13.322271000	3.286859711	11.046737850	N	18.191440673	6.128751590	6.929176755
H	13.677764944	4.996449201	10.715977507	N	19.992608508	5.203850073	10.612577485
C	13.970888291	4.523610740	13.413066119	N	20.876858689	3.240592332	10.313852585
H	13.479282572	5.480535164	13.209118773	N	17.587771508	5.819761649	11.169630562
H	13.188650886	3.765708390	13.513807695	N	15.856901494	4.566842621	11.583706790
H	14.493128064	4.591897987	14.373219806	C	17.022949012	1.113117959	7.559549022
C	15.554806908	2.748554975	12.618002204	C	16.787580050	0.013282449	8.549632186
H	14.769087400	2.003978834	12.786841312	C	15.538003732	-0.524397736	8.949180950
H	16.190486565	2.395927449	11.802329367	C	14.290331493	-0.138023560	8.375723359
H	16.156508194	2.826661849	13.530222779	C	15.491333357	-1.523445867	9.967484862
C	17.287197591	4.992467752	6.070324926	C	13.098101961	-0.716531789	8.788786791
C	15.858393289	4.660351898	6.533359677	C	14.295208736	-2.095197450	10.371024578
H	15.360347557	4.037061362	5.783349484	C	13.083338879	-1.699335929	9.787249460
H	15.878744531	4.123559585	7.483311567	H	14.270028489	0.629239776	7.609119317
H	15.273523028	5.577031078	6.663127172	H	16.424948202	-1.837539975	10.428664999
C	18.118671870	3.709833243	5.888287558	H	12.164173295	-0.397628019	8.331910222
H	18.171945701	3.159562031	6.830990517	H	14.298221932	-2.854600182	11.149324270
H	17.662689959	3.066111353	5.127078544	H	12.145988491	-2.145321166	10.107284664
H	19.137240436	3.954256678	5.566617579	H	16.175685898	1.230865422	6.862348446

H 17.666648907 -0.321834535 9.095418711
 C 14.870745646 3.444129259 11.526974708
 C 14.185400805 3.457937253 10.148429353
 H 14.921827595 3.342008268 9.350305903
 H 13.469198973 2.633181738 10.077268586
 H 13.649010855 4.401040739 9.996268307
 C 13.810686124 3.627548874 12.625571018
 H 13.240296553 4.553298775 12.497190926
 H 13.103727650 2.795262845 12.569620157
 H 14.253460168 3.621317758 13.626892393
 C 15.617404226 2.120950261 11.761262683
 H 14.911304268 1.285320453 11.744620344
 H 16.361616362 1.946798061 10.981671607
 H 16.121550296 2.133915508 12.733769282
 C 17.669987652 5.424728933 5.716826358
 C 16.228203979 4.963393527 5.992601802
 H 15.818495468 4.488037477 5.094735814
 H 16.204518517 4.240568117 6.810631719
 H 15.592683951 5.817273705 6.250197719
 C 18.579347460 4.220058422 5.416351289
 H 18.553321725 3.511757253 6.247506905
 H 18.234515619 3.708917159 4.510892255
 H 19.612265088 4.546682893 5.254123895
 C 17.674165653 6.386455942 4.517063239
 H 18.686497112 6.693356078 4.234734542
 H 17.237795473 5.872297430 3.656309440
 H 17.074401387 7.281521240 4.711427560
 C 21.038386254 1.791063304 9.990654701
 C 20.932230937 1.607060994 8.465519736
 H 21.720004231 2.170844724 7.954260610
 H 21.043076957 0.548655540 8.205512649
 H 19.962328890 1.956252038 8.104309001
 C 19.940304195 1.00553977 10.721224828
 H 18.947578525 1.305482445 10.385409023
 H 20.061176396 -0.069198599 10.519611426
 H 20.006745637 1.157170625 11.802943172
 C 22.412862616 1.299855775 10.472685722
 H 22.543076992 1.450737977 11.549170380
 H 22.491377086 0.227509536 10.273332938
 H 23.236021277 1.791196843 9.944478390
 H 17.881739981 0.857439523 6.909461143

¹a (R=ⁱBu)

Fe 18.065648704 3.664838649 9.424765763
 B 18.955598918 6.377268815 10.567324176
 C 18.777983428 7.494969201 8.138926417
 H 19.198561880 8.444955945 8.420408763
 C 18.368575031 7.059631143 6.923137826
 H 18.340610445 7.577242226 5.981146953
 C 18.105843713 5.361592021 8.392023244
 C 21.451234480 5.472224021 10.892656281
 H 21.873512161 6.416501033 11.190579070
 C 22.058112989 4.275271924 10.709922669
 H 23.086814348 3.997082913 10.853079126
 C 19.871776724 4.030010900 10.187984833
 C 17.027145382 6.291273965 12.371639479
 H 17.298376220 7.231817439 12.820956137
 C 16.025750058 5.434396692 12.679991126
 H 15.275073176 5.499964080 13.446827255
 C 17.168858193 4.560738795 10.938451345
 C 19.303598733 7.793319924 11.278998783
 H 18.655113186 8.990277274 10.912151628
 H 17.938188150 8.985536307 10.097123922
 C 18.872321437 10.194268830 11.585915699
 H 18.354451048 11.094026262 11.262354521
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 C 14.425264033 0.426945808 7.638471407
 C 14.485723979 -1.095307571 9.532449122
 C 13.064935774 0.190309817 7.506360770
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 C 12.400281684 -0.684250724 8.376410703
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 H 15.042064327 -1.595219304 10.321920912
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 H 11.334191992 -0.861420101 8.268075178
 H 17.023846769 1.135715633 7.074482026
 H 17.043289979 -0.497235498 9.694915599
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 H 15.208480038 2.994760766 9.614324909
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 H 16.763205532 1.779235294 11.285275684
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³a-TS (R=ⁱBu)

Fe 17.372389311 3.985315005 9.765974666
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 H 21.393363598 11.304303704 11.939948578
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 H 16.261183389 0.907173069 7.657185126
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¹a-TS (R=ⁱBu)

Fe 17.343342106 3.912066339 9.907939333
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 H 19.409220902 6.263329207 5.701706951
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 H 15.158657174 7.772430317 12.734643224
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 N 15.643029786 5.973664932 11.606405684
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 C 16.835000123 -1.065744807 8.275881358
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H	14.086237050	2.557105024	8.866624671	H	20.949799925	7.216767070	12.603840129
C	17.628961765	4.125002938	6.232712408	N	16.893946254	2.167935199	9.140344146
C	18.186769232	2.721232972	6.523580416	N	18.692365559	6.563433137	9.009879138
C	17.944848568	4.488823394	4.771193479	N	17.881834565	5.841306969	7.128499809
H	17.598406457	5.495108723	4.515596686	N	20.147228286	5.387933151	10.673216299
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H	17.422345228	3.783323211	4.118983767	N	17.834102674	6.235125462	11.405555510
H	19.274378380	2.707855611	6.395359396	N	16.083729735	5.235429763	12.222372382
H	17.751458326	1.991845937	5.831514003	C	16.998657925	1.163645933	8.114007989
H	17.950023025	2.412962935	7.542731258	C	16.501650310	0.815860550	9.484760359
C	19.711247969	1.597979078	11.504070966	C	15.066273818	0.461123634	9.714722855
C	18.483078551	1.418139094	12.413123117	C	14.027629820	1.130953054	9.051606891
C	20.916541512	0.882900890	12.137288205	C	14.733114862	-0.573932487	10.598117750
H	21.813826862	0.956609288	11.514094504	C	12.698444327	0.767927858	9.258656082
H	21.145774734	1.268855180	13.135726513	C	13.401852719	-0.936413144	10.812674734
H	20.673485297	-0.178250861	12.239675829	C	12.377931431	-0.267452135	10.141818878
H	18.678443062	1.837247044	13.406377532	H	14.275343980	1.950839406	8.383429489
H	18.253420654	0.353436620	12.521505499	H	15.527991810	-1.100000996	11.123480387
H	17.611465945	1.916216698	11.983567033	H	11.906864764	1.297069695	8.733455362
C	14.324751160	5.278660243	11.712367347	H	13.165592171	-1.740099597	11.505871714
C	14.531241074	3.921488050	12.406882053	H	11.340517628	-0.546422232	10.306311947
C	13.738886355	5.144778815	10.295736789	H	16.274852877	1.176131710	7.292083009
H	13.521632780	6.137396554	9.885785000	H	17.184090388	0.231853885	10.115101517
H	14.448546833	4.647083676	9.635552905	C	14.986451357	4.242126401	12.419137407
H	12.805228303	4.572836245	10.321685022	C	14.137177115	4.188359242	11.138136320
H	13.579401758	3.382210030	12.464144030	H	14.740660825	3.869296823	10.285942576
H	14.897769601	4.076557849	13.427636096	H	13.316748652	3.474126709	11.258170004
C	16.106016153	4.187940288	6.440613566	H	13.713417533	5.174923990	10.920414595
H	15.731425010	5.188470963	6.198667138	C	14.101847533	4.669470996	13.601070349
H	15.610096727	3.467771124	5.780401256	H	13.612121505	5.631891742	13.420352987
H	15.852109896	3.958829614	7.477046665	H	13.316776750	3.920699996	13.738680731
C	19.461995483	1.010294457	10.105909914	H	14.669500675	4.732284173	14.535255306
H	20.325064506	1.190955208	9.455975016	C	15.612535872	2.870978894	12.727087245
H	19.295487205	-0.068851754	10.173472012	H	14.827896702	2.120388354	12.862900749
H	18.574799158	1.455101844	9.651335802	H	16.255596498	2.541630715	11.908848532
H	15.256322834	3.313488497	11.864882883	H	16.212780832	2.921044554	13.642075339
C	13.348195934	6.110159969	12.564185094	C	17.203228955	4.981611214	6.113615255
H	13.138423974	7.088338348	12.120211632	C	15.836073388	4.538371023	6.662742936
H	12.400292727	5.567443892	12.624202491	H	15.312112592	3.949369235	5.902263620
H	13.711383933	6.254478190	13.586624506	H	15.943213016	3.924129816	7.559684209

⁵²(R="Bu)

Fe	17.740446794	3.802783020	9.756245856
B	19.105266215	6.577509058	10.535361462
C	19.055325963	7.471925476	8.028316919
H	19.650724614	8.345864508	8.230191045
C	18.541923857	7.033376238	6.851617883
H	18.588117908	7.474592561	5.871275801
C	17.996772147	5.531312947	8.453204429
C	21.522387387	5.470895932	10.824670067
H	22.046314198	6.406157653	10.923324951
C	22.016937690	4.206213808	10.807483182
H	23.029105036	3.858528399	10.921155906
C	19.781143654	4.087451777	10.501975874
C	17.332484766	7.037686728	12.424518740
H	17.787282719	7.971393713	12.707355074
C	16.239341436	6.422322682	12.934388796
H	15.586100930	6.725538312	13.733738041
C	17.058171396	5.117362974	11.277268827
C	19.680902531	8.015030277	11.043347432
C	19.172073285	9.236015440	10.554871265
H	18.411551701	9.228089700	9.779602215
C	19.587704482	10.473749683	11.052026015
H	19.170022491	11.387637920	10.636445838
C	20.524385076	10.538819412	12.083852811
H	20.855175680	11.498948769	12.470835624
C	21.007925942	9.349198612	12.628911820
H	21.711505319	9.375536025	13.457687866
C	20.582503601	8.118363324	12.122767877

⁵²(R="Bu)

Fe	17.794506264	3.842825865	9.830575859
B	19.061976004	6.600938799	10.509057257
C	19.003100737	7.489996850	7.999715860
H	19.549593072	8.394111664	8.205182729

C	18.538936990	7.017816979	6.816932290	H	16.631104132	5.028048648	4.023397585
H	18.587107717	7.452766316	5.833900011	H	16.550842140	6.583006655	4.862145655
C	18.036596369	5.493122330	8.421122810	C	20.805021169	1.845338762	10.545985046
C	21.440958390	5.427252913	10.823492023	C	20.534907810	1.423725141	9.091855475
H	21.998503558	6.342972199	10.920279308	H	21.297817425	1.836639582	8.423204011
C	21.883895561	4.146033358	10.813520503	H	20.554365214	0.332059292	9.004248363
H	22.880113396	3.759981261	10.937808074	H	19.554877212	1.784133412	8.774888356
C	19.646111110	4.113819895	10.488795794	C	19.741686204	1.271900361	11.498057609
C	17.223571278	7.062188412	12.342783711	H	18.743726427	1.610559587	11.214425692
H	17.595920135	8.047263632	12.567471104	H	19.762699889	0.177516237	11.461355094
C	16.188337052	6.380851109	12.889708010	H	19.937893983	1.587047791	12.528199117
H	15.504654421	6.670537012	13.668118256	C	22.188739557	1.332282581	10.977575647
C	17.121946084	5.066708690	11.304604776	H	22.444856045	1.655824649	11.991454962
C	19.632485671	8.036637210	11.022041195	H	22.172667845	0.238803882	10.969347272
C	19.102982738	9.254046311	10.544823231	H	22.981125953	1.651562302	10.293224932
H	18.327679374	9.239894017	9.784531012	H	17.914312005	0.973885261	7.601882404
C	19.518801636	10.494746810	11.032982025	*****			
H	19.086323355	11.405555611	10.625545592	12 (R=ⁿBu)			
C	20.477099018	10.566596821	12.044693370	*****			
H	20.810226176	11.529353570	12.423215259	Fe	17.740416952	3.873820330	9.819837339
C	20.979411362	9.380753368	12.580446844	B	19.121633700	6.606313716	10.554160221
H	21.699697941	9.412486586	13.394510186	C	18.932713641	7.423035897	8.050471839
C	20.552308604	8.146532328	12.083999331	H	19.506221197	8.320400846	8.205259819
H	20.934737060	7.248552160	12.559337312	C	18.375050750	6.938605421	6.918246319
N	16.997231733	2.256217590	9.130904238	H	18.352109444	7.360846633	5.930405912
N	18.663204192	6.572008563	8.980861373	C	17.990194088	5.432651133	8.580296969
N	17.930219930	5.797120847	7.090766370	C	21.448936174	5.341990817	10.907827218
N	20.066676311	5.398895696	10.664655777	H	22.048308172	6.228990027	11.019744264
N	20.766886757	3.335655476	10.626032335	C	21.826202986	4.040501763	10.906653724
N	17.795131071	6.250437408	11.374714260	H	22.798317672	3.605560127	11.055825702
N	16.138139696	5.145557149	12.247527577	C	19.595509771	4.123303286	10.492587249
C	16.968735601	1.346290654	8.009477029	C	17.311873460	7.035016506	12.440432725
C	16.551544117	0.884358781	9.367581871	H	17.730906789	7.972804873	12.765610922
C	15.122358617	0.566232333	9.665107893	C	16.224801220	6.361230309	12.888648408
C	14.064142498	1.266592356	9.066845443	H	15.534347106	6.609755259	13.675068882
C	14.812867047	-0.477615041	10.547511551	C	17.149239682	5.154835442	11.204256549
C	12.740359018	0.926488787	9.337878847	C	19.718785945	8.042106777	11.029994284
C	13.487747257	-0.816929872	10.825842733	C	19.186281057	9.257643532	10.551879651
C	12.444331059	-0.116609710	10.220265665	H	18.396198091	9.240685457	9.806966734
H	14.285810591	2.091388603	8.395553953	C	19.617349523	10.500694554	11.020761088
H	15.622426181	-1.030476697	11.019877807	H	19.180744064	11.410122167	10.614561207
H	11.934460440	1.479620256	8.861682108	C	20.595173356	10.577213794	12.013127600
H	13.272019883	-1.629095179	11.515665777	H	20.939614192	11.541806091	12.376760450
H	11.411349643	-0.378812186	10.432673918	C	21.103053175	9.394119124	12.549308221
H	16.195114860	1.474831987	7.247545695	H	21.839695704	9.430096073	13.348526989
H	17.248344481	0.229014822	9.899664786	C	20.660924989	8.157316786	12.072071162
C	15.104805099	4.097739323	12.494356254	H	21.048454053	7.262482037	12.548552098
C	14.139566723	4.083174169	11.296583311	N	17.145265308	2.338615403	8.839306749
H	14.677044406	3.848452126	10.375580553	N	18.661886928	6.525313417	9.062107312
H	13.362481264	3.326074211	11.440066058	N	17.773301203	5.726973085	7.245743784
H	13.657898199	5.061127169	11.184344804	N	20.084237886	5.379185428	10.701074976
C	14.328061900	4.425596380	13.779413734	N	20.678979380	3.288520891	10.670527822
H	13.739940135	5.344141944	13.686391784	N	17.864206327	6.287985500	11.417497257
H	13.628498795	3.609611651	13.980469816	N	16.128360737	5.198564990	12.124874898
H	14.994171833	4.518546813	14.643319827	C	17.075925044	1.362405310	7.784208863
C	15.802297931	2.739315018	12.668132790	C	16.775055308	0.948030722	9.182163596
H	15.056272056	1.956677223	12.836238392	C	15.383065400	0.581472120	9.584670452
H	16.372742693	2.476440191	11.776533605	C	14.255991523	1.215193376	9.039038256
H	16.483588838	2.765802264	13.525576830	C	15.178786797	-0.449337820	10.512235675
C	17.307915519	4.912063840	6.063647494	C	12.969637253	0.824981666	9.406370399
C	15.915936666	4.483127683	6.558026261	C	13.891534311	-0.838754440	10.886984407
H	15.448261914	3.824473656	5.817967242	C	12.779587043	-0.203069247	10.334380485
H	15.980614120	3.955365136	7.511041055	H	14.393642205	2.025560808	8.329704416
H	15.274610295	5.361273430	6.689231709	H	16.041605866	-0.952600679	10.944013104
C	18.231442040	3.700781018	5.844815444	H	12.109818614	1.326132231	8.968199285
H	18.385968007	3.162978608	6.780786132	H	13.758945444	-1.639066531	11.610771929
H	17.792869359	3.011754233	5.114922222	H	11.775766748	-0.503232639	10.622627869
H	19.206387415	4.027699130	5.466918237	H	16.247534932	1.414133241	7.071143872
C	17.148867324	5.674657605	4.737649674	H	17.532293405	0.339049120	9.684467841
H	18.112508163	5.944265025	4.293851779	C	15.033096504	4.195554662	12.244113270

C	14.166719990	4.267524873	10.974826453
H	14.764351274	4.049704277	10.086935348
H	13.352935718	3.538049940	11.025807545
H	13.735741531	5.269112449	10.868140074
C	14.160333665	4.506189838	13.471501097
H	13.647662643	5.468818416	13.378882868
H	13.392479923	3.732350410	13.557761246
H	14.743152677	4.504400679	14.398305469
C	15.657563548	2.802687186	12.424403408
H	14.876521164	2.043408445	12.524478877
H	16.265782335	2.530434921	11.558796068
H	16.290533032	2.779487617	13.318017791
C	17.087092914	4.884953492	6.217732269
C	15.738752302	4.403978388	6.777082643
H	15.229119497	3.789489232	6.026813417
H	15.875848482	3.815625399	7.684385232
H	15.100339999	5.265551455	7.002325798
C	18.035258954	3.733383545	5.841148239
H	18.349869087	3.191333063	6.730735858
H	17.543784608	3.035851307	5.154634841
H	18.926282423	4.132513373	5.343901139
C	16.794732679	5.715987191	4.952455245
H	17.704046660	6.017474785	4.423944502
H	16.214140884	5.094968979	4.264260671
H	16.202417734	6.608472330	5.177995131
C	20.660028537	1.796456660	10.628722015
C	20.436513400	1.342294240	9.176613622
H	21.264431930	1.678575322	8.543300726
H	20.385803561	0.249274470	9.123599958
H	19.505903997	1.766640073	8.795534424
C	19.542144198	1.296834492	11.559483327
H	18.567340584	1.664437155	11.236152765
H	19.511945762	0.202137692	11.558306367
H	19.716726990	1.636943192	12.585454364
C	21.998599053	1.233996832	11.137123357
H	22.223456204	1.568740592	12.154752730
H	21.933301274	0.142235619	11.150222980
H	22.834147979	1.501869927	10.483161831
H	18.008656875	1.010278219	7.329797747

51 (R=H)

Fe	17.124757957	3.949636454	10.014684486
B	18.916369791	6.526390069	10.625876687
C	19.642850740	6.686393158	8.039134393
H	20.368459613	7.469314772	8.178438513
C	19.343183190	5.975303626	6.917647430
H	19.728709889	6.039032481	5.912741673
C	18.068925797	5.191637202	8.616245234
C	20.834641033	4.974776565	11.710505368
H	21.554864470	5.764090657	11.842090893
C	20.969955586	3.637175598	11.923455423
H	21.801440408	3.058110111	12.292021688
C	18.889248843	4.020305686	11.123356552
C	16.892702830	7.736269461	11.836988937
H	17.467279439	8.619925773	12.056555607
C	15.596065741	7.448511799	12.122434714
H	14.834975418	8.019538162	12.629325793
C	16.493460077	5.672536197	11.020121204
C	19.720677224	7.882130391	11.001638257
C	19.697230632	9.018525299	10.168286785
H	19.164871105	8.979987353	9.222621290
C	20.318182277	10.217985553	10.524754505
H	20.280028816	11.066688089	9.846873678
C	20.976981153	10.330995527	11.749206719
H	21.465158739	11.260185431	12.028910378
C	20.979421641	9.239705061	12.618414638
H	21.461638330	9.317818707	13.589264963
C	20.354833553	8.045782178	12.249595959
H	20.345508448	7.231108486	12.967321936

N	17.220432143	2.464131595	9.315595050
N	18.837822800	6.217895782	9.071416560
N	18.372408119	5.067338008	7.305068434
N	19.545898422	5.205011661	11.242034276
N	19.757383416	3.079591491	11.554823568
N	17.434633450	6.646644488	11.164409343
N	15.380181728	6.177753894	11.610012988
H	14.509859928	5.670968927	11.656314933
H	19.531741704	2.096348944	11.519129257
H	17.972583266	4.336179859	6.735636128

31 (R=H)

Fe	17.194048058	3.974386224	9.959026281
B	19.006950494	6.490708579	10.635345669
C	19.632572497	6.670651456	8.008336273
H	20.332799623	7.482447934	8.107021444
C	19.277692716	5.963320351	6.902078002
H	19.580754968	6.057000996	5.871799513
C	18.157758667	5.115470531	8.678112557
C	20.889970261	4.945997925	11.811799013
H	21.600149420	5.735107176	11.990636636
C	21.002177844	3.612444109	12.054446382
H	21.798544404	3.035461437	12.496719092
C	18.975050530	3.994273566	11.097125179
C	16.897055317	7.569537481	11.865845489
H	17.417835153	8.464228698	12.163173337
C	15.607168928	7.196518511	12.073674949
H	14.795533237	7.694611380	12.578532292
C	16.641549062	5.549542852	10.917638926
C	19.765633578	7.871285886	11.011517836
C	19.700136030	9.002863157	10.173452049
H	19.163392638	8.943131994	9.231823578
C	20.280473415	10.224933970	10.521355280
H	20.210010048	11.068472280	9.839747099
C	20.939408645	10.366856483	11.742901149
H	21.396849245	11.313599564	12.016292589
C	20.981302396	9.281183340	12.617810236
H	21.462863857	9.381750210	13.587019307
C	20.396519550	8.064275029	12.257514760
H	20.416823072	7.255834118	12.981548917
N	15.885919599	3.317920120	9.434798247
N	18.921179732	6.163509030	9.088432595
N	18.362171068	5.019367613	7.342557572
N	19.641163246	5.172151359	11.248912180
N	19.811099610	3.056569404	11.612096149
N	17.524140384	6.554386886	11.150626262
N	15.476744556	5.947612275	11.478759289
H	14.642269047	5.383535155	11.432694060
H	19.581810018	2.074808712	11.630081304
H	17.907482635	4.318584062	6.777956727

11 (R=H)

Fe	17.297479153	4.071696825	10.005012146
B	18.968956652	6.508363946	10.602600360
C	19.580442332	6.712898330	7.968164230
H	20.271939585	7.532298692	8.068310902
C	19.236885280	6.005662388	6.861610358
H	19.543125050	6.101948732	5.832103337
C	18.133679277	5.125291305	8.633475213
C	20.819686896	4.924572586	11.796383103
H	21.538256835	5.703303732	11.988348876
C	20.909642094	3.591086284	12.033850720
H	21.691564390	2.999183797	12.482405248
C	18.915338056	3.998339308	11.039325982
C	16.860535999	7.632802268	11.810389722
H	17.383578171	8.539850658	12.065555283
C	15.576915741	7.266915479	12.053650372
H	14.771558283	7.781793340	12.552696753

C	16.592099750	5.576253939	10.939885191
C	19.744526425	7.872879750	10.989987167
C	19.704103900	9.013533400	10.163243249
H	19.174781102	8.973109055	9.215835227
C	20.301180265	10.221945975	10.530224639
C	20.252421001	11.074403799	9.856791692
C	20.949534667	10.338995118	11.759569827
H	21.420916705	11.275383991	12.047389057
C	20.965614351	9.244110664	12.623687232
H	21.439745441	9.327036576	13.598845680
C	20.364056324	8.041842623	12.244895096
H	20.363093437	7.224170561	12.959543445
N	16.499079704	2.849781641	9.691796088
N	18.879297203	6.191057801	9.052113988
N	18.339363086	5.036145067	7.297428531
N	19.581520254	5.178882138	11.212222755
N	19.720513059	3.043235360	11.563400595
N	17.482334923	6.591528447	11.126546647
N	15.435679446	5.993179830	11.506017932
H	14.598533981	5.432791460	11.514716470
H	19.472767916	2.066725466	11.570809836
H	17.903596245	4.330125516	6.725873883

⁵¹a (R=H)

Fe	18.208881187	2.822767661	8.852914146
B	18.210709960	5.680735609	10.328300004
C	18.901451540	6.992667728	8.080066278
H	19.028390214	7.954131413	8.548079964
C	19.120310401	6.627083960	6.788807752
H	19.440543990	7.199460625	5.932396657
C	18.461579970	4.786135971	7.947835789
C	20.530763464	5.085717322	11.556998855
H	20.667809487	6.058776877	11.997429317
C	21.349389327	4.000432952	11.588671973
H	22.299583279	3.838881492	12.072740063
C	19.530703524	3.489101593	10.326226258
C	15.735187010	5.239968437	11.182382519
H	15.657772998	6.193139680	11.677317478
C	14.832795584	4.231018762	11.084198345
H	13.832015252	4.131241719	11.473485826
C	16.705375438	3.608631640	9.972521111
C	18.062040092	7.062665646	11.163138035
C	17.462606596	8.209737817	10.605240148
H	17.136067859	8.195629084	9.569611876
C	17.239175257	9.371019821	11.348816716
H	16.780482327	10.235299831	10.874616306
C	17.592181430	9.419098872	12.697520881
H	17.423394287	10.321409988	13.279651566
C	18.142323074	8.284988802	13.294129748
H	18.393749285	8.293239593	14.352011328
C	18.360656852	7.130807940	12.538960781
H	18.752266327	6.254886793	13.047899939
N	17.964557427	1.449835029	7.795609656
N	18.475784047	5.866882123	8.776273591
N	18.837453841	5.270509112	6.739298689
N	19.409670446	4.755890035	10.806139994
N	20.707689623	3.034788505	10.828384342
N	16.885969254	4.850524932	10.500292991
N	15.454468885	3.241744127	10.334779849
H	15.044656423	2.353117028	10.075931614
H	21.065872770	2.114412441	10.626598821
H	18.913510189	4.680803786	5.924710176
C	17.432284533	0.113963256	7.809856774
C	17.034389985	-0.357897675	9.184875311
C	15.740468621	-0.275656404	9.753281661
C	14.598021301	0.190545189	9.030142069
C	15.523671036	-0.660583090	11.112204592
C	13.345561020	0.257516722	9.629424087
C	14.269980220	-0.590275053	11.697410589

C	13.165102959	-0.131243807	10.963785397
H	14.712168887	0.502204790	7.997068619
H	16.373386062	-1.012770073	11.691909071
H	12.496566078	0.614882618	9.051687546
H	14.144082293	-0.889375754	12.734817237
H	12.182858826	-0.077000577	11.423856392
H	16.592713346	0.024778629	7.100029257
H	17.844228088	-0.673588210	9.840918195
H	18.208268029	-0.560349022	7.406917125

³¹a (R=H)

Fe	18.084736822	3.017575992	8.561832687
B	18.166093866	5.685814300	10.322997989
C	18.718399970	7.152840558	8.108927694
H	18.860484166	8.096353154	8.609087847
C	18.860653666	6.842882297	6.790833196
H	19.116692426	7.454099656	5.939883944
C	18.309968915	4.945613915	7.917360823
C	20.493223727	4.786799712	11.384570240
H	20.709065784	5.654361524	11.985218594
C	21.232601805	3.661570482	11.193742501
H	22.180248930	3.354542096	11.606896792
C	19.354630565	3.504701965	9.929514215
C	15.701986143	5.097646721	11.167251259
H	15.606132676	5.962655048	11.802582823
C	14.830595279	4.082898848	10.924121750
H	13.842097741	3.885577095	11.306800987
C	16.709201111	3.700209402	9.719091270
C	18.084857437	6.966401001	11.303691524
C	17.506735136	8.186511180	10.899850163
H	17.135352781	8.295975053	9.885063376
C	17.361445420	9.267153539	11.773497212
H	16.913651367	10.192160547	11.418403178
C	17.779044298	9.158083269	13.099802070
H	17.672183811	9.997430391	13.782163802
C	18.313911591	7.949075583	13.544619149
H	18.616494454	7.836290690	14.582962499
C	18.452364483	6.876364146	12.661441990
H	18.835937306	5.938532385	13.052239505
N	18.063563841	1.392289708	8.325404880
N	18.361298652	5.995400323	8.780673936
N	18.598150243	5.484704497	6.702240439
N	19.334347465	4.671232884	10.627861460
N	20.506369735	2.886449525	10.300504086
N	16.848517551	4.852464810	10.423868944
N	15.471447352	3.239704348	10.027943226
H	15.110633225	2.361026911	9.679305424
H	20.780894201	1.993848262	9.921575387
H	18.639772968	4.931922673	5.859925126
C	18.020668093	-0.001251968	8.747749360
C	17.321602930	-0.161553452	10.063272789
C	15.915712447	-0.127967742	10.235135365
C	15.010379089	0.003013615	9.139110491
C	15.343327533	-0.209790392	11.538453189
C	13.636551827	0.048873855	9.346655710
C	13.971189269	-0.168707453	11.732061382
C	13.101773079	-0.037109524	10.639495991
H	15.407048309	0.089058229	8.132686723
H	16.008592661	-0.304321715	12.392849271
H	12.971358995	0.156798231	8.493415102
H	13.568762202	-0.230595130	12.740077603
H	12.027442414	0.003145538	10.793597479
H	17.528169948	-0.598610627	7.963394798
H	17.933397840	-0.142660561	10.962842548
H	19.046620141	-0.397323889	8.825147403

¹a (R=H)

Fe	18.160899429	3.101148446	8.329282864
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B	18.183361164	5.617627499	10.323405465
C	18.910339300	7.251196830	8.284794337
H	19.038276101	8.144952317	8.872469448
C	19.127256679	7.051683728	6.955648227
H	19.446025835	7.727528289	6.177828616
C	18.465374945	5.080576278	7.877009469
C	20.405856863	4.567524098	11.465202110
H	20.594423881	5.375911405	12.151486375
C	21.132505889	3.440934419	11.233969408
H	22.040010598	3.074789646	11.687128901
C	19.352368914	3.445055902	9.825767711
C	15.663715856	5.022824864	10.959750588
H	15.547607606	5.834586612	11.659182223
C	14.787964766	4.056390921	10.579911417
H	13.774268024	3.852240534	10.885008106
C	16.726274011	3.732290755	9.448110608
C	18.058479186	6.817985222	11.398348624
C	17.527794686	8.078412565	11.057666766
H	17.230396534	8.277911178	10.032247409
C	17.335387835	9.087219244	12.004979548
H	16.927096084	10.046672652	11.696766947
C	17.654030259	8.861914630	13.344254801
H	17.509328698	9.644436110	14.084757638
C	18.140544454	7.610959041	13.723475186
H	18.366595922	7.407961398	14.767516490
C	18.327902965	6.611378617	12.766557175
H	18.670383805	5.638038550	13.105412307
N	17.954324355	1.525618487	7.910569543
N	18.486023562	6.050440509	8.829911095
N	18.840746342	5.713681797	6.733286770
N	19.306944702	4.549354443	10.617290707
N	20.459118367	2.765197752	10.226502858
N	16.845470582	4.815817628	10.259552998
N	15.460269190	3.283802786	9.643226360
H	15.110456681	2.428540401	9.235794738
H	20.740904127	1.899017673	9.794666235
H	18.920373632	5.234928440	5.849325469
C	17.537831586	0.153823075	8.165460539
C	17.188531329	-0.042721000	9.609193767
C	15.891247973	-0.039342094	10.176006145
C	14.692385641	-0.029205181	9.398502484
C	15.733935999	-0.019290087	11.595081218
C	13.442509318	0.017240169	10.004341450
C	14.482631287	0.027789619	12.186994376
C	13.321417309	0.051099125	11.399824575
H	14.757969050	-0.068546830	8.315458892
H	16.627329891	-0.024391483	12.214632708
H	12.548887489	0.023396461	9.384947925
H	14.401986485	0.054662731	13.270738954
H	12.341401282	0.089346936	11.866267801
H	16.696951322	-0.101599838	7.503705366
H	18.027843171	-0.021677092	10.301985985
H	18.356552663	-0.529444683	7.877703119

⁵¹TS (R=H)

Fe	17.342282845	3.972346393	9.780445655
B	19.064972265	6.603369283	10.444452365
C	19.600650563	6.995983309	7.836687779
H	20.272031273	7.823572039	7.990865458
C	19.275382997	6.352783801	6.682510479
H	19.581454128	6.524668836	5.662645877
C	18.184042093	5.342090427	8.392530228
C	21.150884429	5.139356123	11.305009784
H	21.821810396	5.971764017	11.433311740
C	21.391680321	3.807795821	11.447475144
H	22.281466909	3.274657870	11.743323266
C	19.237855328	4.073543230	10.787560451
C	17.085379896	7.597058754	11.899186243
H	17.635636929	8.485059649	12.160911184

C	15.825856667	7.220478918	12.245173990
H	15.080908655	7.707726289	12.854306015
C	16.708103451	5.601139565	10.928993129
C	19.796518011	7.994576036	10.843750248
C	19.593353325	9.171753858	10.095252125
H	18.975763028	9.139803278	9.202362360
C	20.135835402	10.401035551	10.475237319
H	19.957508486	11.281969218	9.863400623
C	20.894147956	10.501552588	11.641539352
H	21.322160571	11.455002093	11.939977228
C	21.076110165	9.366317423	12.430979109
H	21.638721645	9.433079693	13.358946413
C	20.527195982	8.142764657	12.039476336
H	20.654365566	7.290930238	12.700981759
N	17.125338875	2.473452890	9.028829181
N	18.907849564	6.387355657	8.877191068
N	18.400212498	5.346750544	7.056773510
N	19.821951644	5.295783240	10.927028116
N	20.197659081	3.182352305	11.128135399
N	17.621035892	6.600304731	11.090162941
N	15.623198109	5.993239844	11.636738910
H	14.764606067	5.456951882	11.667528625
H	20.041236488	2.186846451	11.080729203
H	18.006953873	4.642156838	6.451352066
C	15.397621411	1.227031604	8.741293147
C	14.751067298	1.352373506	9.938823160
C	13.922964363	2.474962146	10.344865139
C	13.659711683	3.584386906	9.507017302
C	13.373013613	2.502490453	11.646542698
C	12.867813382	4.644034326	9.944537718
C	12.590354328	3.565991212	12.086174429
C	12.327060299	4.647049245	11.235987672
H	14.081120920	3.613112526	8.507772053
H	13.572453684	1.669103678	12.316068105
H	12.678384916	5.481031911	9.277121295
H	12.180759856	3.553899706	13.093255196
H	11.706219740	5.473609618	11.571187680
H	15.969014790	0.332770677	8.525873693
H	14.963184954	0.620868771	10.716780719
H	15.134507712	1.830014363	7.881108491

³¹TS (R=H)

Fe	17.659201321	3.441783694	8.914120642
B	18.571567286	6.187802839	10.215105007
C	19.292319346	7.172276022	7.799347619
H	19.712875738	8.094235692	8.164387610
C	19.239717258	6.689410285	6.528186583
H	19.573484213	7.110086599	5.592818748
C	18.307340034	5.150632662	7.916120232
C	20.693798791	4.884932071	11.282284832
H	21.165948284	5.750560962	11.715285261
C	21.114726096	3.592456504	11.254653017
H	21.989445845	3.120310611	11.672527614
C	19.159593896	3.728738061	10.118425933
C	16.143116235	6.396571856	11.295092125
H	16.339794620	7.340735171	11.775681500
C	15.022366208	5.627558076	11.291646344
H	14.064538168	5.758131610	11.768838814
C	16.586522333	4.586950682	10.039402394
C	18.895914161	7.572943590	10.984766724
C	18.578473832	8.826982738	10.424373860
H	18.144013400	8.878136676	9.430299478
C	18.771051419	10.024040759	11.118008422
H	18.516770047	10.969316261	10.644746928
C	19.276764916	10.007510582	12.417673360
H	19.432075456	10.936292635	12.960523606
C	19.557692360	8.781331018	13.019805922
H	19.922588582	8.748426874	14.043463586
C	19.359675113	7.591462987	12.315634619

H	19.548346737	6.655430271	12.832707648	C	14.239283769	1.494429303	9.971874488
N	17.149901858	1.958334098	8.929717293	C	14.046048944	2.618498871	9.132641609
N	18.699805506	6.237148685	8.634366216	C	13.409915368	1.387396001	11.114604292
N	18.625721354	5.450857895	6.630503855	C	13.075601924	3.571409739	9.421630567
N	19.481859946	4.956065668	10.606596027	C	12.439921124	2.344514245	11.399885482
N	20.148946035	2.901420529	10.536586970	C	12.265122301	3.444288700	10.554214763
N	17.100319117	5.747742662	10.523590611	H	14.676748031	2.752598688	8.260980003
N	15.320221581	4.523727432	10.507744730	H	13.541750110	0.536112103	11.778290672
H	14.710930411	3.727749708	10.355406051	H	12.955093608	4.428556491	8.764472535
H	20.154697179	1.917183273	10.319437069	H	11.818728726	2.234720622	12.285091104
H	18.449299406	4.820610739	5.863375570	H	11.511214486	4.194101414	10.776606612
C	16.331361679	0.348992702	9.904530653	H	16.101354687	1.202259261	7.886560349
C	15.804714566	0.729951413	11.121907556	H	15.360213280	-0.275107914	10.489930640
C	14.511941382	1.343961096	11.331660147	H	16.912891795	-0.251790643	8.621475909
C	13.608255005	1.640319067	10.278388961	*****			
C	14.111220295	1.713008255	12.639075697	11-TS (OSS) (R=H)			
C	12.385319231	2.260852384	10.527975304	*****			
C	12.890577562	2.332030080	12.882666252	Fe	18.067248000	3.090840335	10.017095672
C	12.013539657	2.614792428	11.829319905	B	18.563733955	6.085445351	10.483694065
H	13.878672748	1.391321870	9.256966512	C	18.311689228	6.490143750	7.810570493
H	14.786087843	1.509063526	13.467097202	H	18.519303262	7.546816468	7.823188383
H	11.718341776	2.476753603	9.696620597	C	18.091644225	5.667880752	6.752951819
H	12.620985541	2.603186189	13.900577411	H	18.046462756	5.866773972	5.694148673
H	11.061429340	3.102187678	12.018005800	C	18.020727867	4.422397474	8.648874753
H	15.685497164	0.170197746	9.050969709	C	21.167822288	5.596825809	11.037665788
H	16.449680987	0.681534991	11.997765063	H	21.462788541	6.626238187	11.150849887
H	17.260650497	-0.211016129	9.886041963	C	21.926471341	4.472209580	11.088033448

11-TS (CSS) (R=H)

Fe	17.979966586	3.154033931	9.953515298	H	22.978613599	4.331589795	11.277788425
B	18.573957664	6.131462478	10.463828866	C	19.786975608	3.863173282	10.623020339
C	18.425740260	6.567146206	7.786972983	C	16.552689397	6.078735727	12.253938018
H	18.675890903	7.6144431595	7.810606051	H	16.645629792	7.122997389	12.503398067
C	18.204792057	5.757728132	6.719757624	C	15.674033501	5.145771659	12.702401951
H	18.199032193	5.961608246	5.660849083	H	14.858897463	5.215724774	13.404502503
C	18.027340437	4.508980156	8.608942479	C	17.063950690	4.147523914	11.225355055
C	21.131652280	5.517787336	11.116495754	C	18.663598173	7.667840537	10.803917089
H	21.467773991	6.530610987	11.261279583	C	17.835022790	8.595739511	10.140005845
C	21.835970868	4.358702288	11.180805844	H	17.152143380	8.249649719	9.369741548
H	22.871524634	4.167138242	11.412943946	C	17.832092350	9.955471003	10.457513043
C	19.692786182	3.856457146	10.612967192	H	17.179718143	10.635395370	9.914917646
C	16.494340414	6.176129252	12.153925669	C	18.654558513	10.438787868	11.475044878
H	16.615311032	7.211830924	12.425347833	H	18.658894156	11.496891622	11.723981260
C	15.566007396	5.267933142	12.550000218	C	19.453056567	9.541570515	12.183570516
H	14.727336156	5.354890889	13.221912792	H	20.077289916	9.896895621	12.999732771
C	16.975846284	4.245822297	11.108888328	C	19.445700392	8.183057251	11.856500367
C	18.736508141	7.700815644	10.818765451	H	20.048298445	7.510349190	12.459002078
C	17.999514763	8.687826819	10.133172941	N	17.541571421	1.653168016	9.723154961
H	17.339474400	8.397449158	9.321168295	N	18.239554899	5.729427766	8.973362642
C	18.058626235	10.039323926	10.480307752	N	17.903588577	4.400018084	7.294894655
H	17.477306140	10.767194856	9.919268965	N	19.854135201	5.220311746	10.778940402
C	18.851647252	10.453851743	11.550246823	N	21.052019322	3.419815152	10.839431818
H	18.904651804	11.505075986	11.822020936	N	17.402357679	5.460016717	11.341810485
C	19.556866914	9.497560452	12.280566006	N	16.014979482	3.960421689	12.060386374
H	20.155352061	9.799589591	13.136639635	H	15.505130981	3.090851091	12.107703565
C	19.488448604	8.148758374	11.923109788	H	21.305790836	2.446393280	10.785164170
H	20.017803114	7.429722480	12.540922464	H	17.773792096	3.548680122	6.772758284
N	17.380931804	1.733192294	9.699291713	C	16.208748725	0.625002100	8.795419556
N	18.289945037	5.805514338	8.942875865	C	15.144935587	0.574194608	9.684246855
N	17.950432618	4.496456806	7.250704167	C	14.183472742	1.632840901	9.898446373
N	19.815688059	5.206304118	10.793795390	C	14.159688034	2.823626822	9.132480406
N	20.926685625	3.351426425	10.876524005	C	13.232064688	1.512044516	10.940217082
N	17.357402365	5.542425070	11.265361959	C	13.231955245	3.826360887	9.394631842
N	15.887036195	4.082572796	11.896952922	C	12.306092944	2.518134160	11.198790834
H	15.348175902	3.228110198	11.914455578	C	12.298465115	3.684648097	10.426539540
H	21.137125614	2.367740756	10.821680666	H	14.888442329	2.969638878	8.342749364
H	17.787855013	3.656423009	6.719598226	H	13.230869020	0.607698959	11.544841307
C	16.262703264	0.603520140	8.777134474	H	13.242090293	4.732835770	8.794988879
C	15.259401362	0.500193191	9.733917682	H	11.587128630	2.393773304	12.004667514
				H	11.577939318	4.472121150	10.627304170
				H	16.158787199	1.272953440	7.926927346
				H	15.120663030	-0.244814185	10.400793587

H 16.801674250 -0.272111680 8.649148686

³¹a-TS (R=H)

Fe 17.476498291 3.932258926 9.710806323
B 19.104468686 6.480392198 10.472921203
C 19.545159769 6.990375690 7.848059678
H 20.165757012 7.857303535 7.998201030
C 19.201389221 6.366838200 6.691156271
H 19.437654847 6.592450282 5.663358345
C 18.281314812 5.217568163 8.419798059
C 21.111199748 4.902376352 11.388124513
H 21.809360234 5.693076845 11.604682437
C 21.275029702 3.556737790 11.485159163
H 22.109720122 2.963762219 11.823754164
C 19.194877483 3.964633337 10.672735804
C 17.017875669 7.363954753 11.883610449
H 17.488099206 8.293480508 12.158882493
C 15.788238256 6.878633664 12.196444095
H 14.987861228 7.293630520 12.787946388
C 16.833930187 5.349995127 10.896895414
C 19.816672636 7.854636153 10.940853455
C 19.612741334 9.064147073 10.246077548
H 18.998694798 9.071608206 9.350244002
C 20.148878970 10.276275728 10.685989529
H 19.971001415 11.184148655 10.114617713
C 20.900890185 10.324842158 11.859877568
H 21.325003177 11.264641417 12.203958256
C 21.080554043 9.155377860 12.598183484
H 21.636868603 9.181039753 13.532081899
C 20.537712373 7.949800747 12.147571071
H 20.661807083 7.069789619 12.771266377
N 16.352628175 2.854455867 9.014699122
N 18.959772180 6.297558036 8.902917060
N 18.417747484 5.284239253 7.071748543
N 19.826167540 5.145917740 10.919202288
N 20.078422035 3.002852420 11.047618043
N 17.656875105 6.418169876 11.088202278
N 15.701000586 5.638502113 11.578641914
H 14.897969894 5.024032367 11.597303895
H 19.880294984 2.018111613 10.965943045
H 18.013052590 4.600149820 6.452692240
C 15.236864999 2.159695446 8.466740892
C 14.560297484 2.099249261 9.787573406
C 13.682450813 3.099786487 10.308565768
C 13.204110315 4.197532544 9.5411337195
C 13.238517080 3.018228923 11.658053804
C 12.331642485 5.131535522 10.086502304
C 12.363305910 3.956439392 12.194372515
C 11.899491870 5.023635164 11.414575789
H 13.541970294 4.320894566 8.517647861
H 13.594460638 2.196770797 12.275489609
H 11.989960194 5.961957831 9.473513233
H 12.043574668 3.860522001 13.229293843
H 11.219917779 5.759153767 11.834849707
H 14.688242722 2.719738801 7.695091636
H 14.894423755 1.318030933 10.462454940
H 15.491602635 1.170409472 8.058124570

¹¹a-TS (R=H)

Fe 17.519339926 3.832616983 9.828602857
B 19.127276108 6.493161766 10.491975083
C 19.527430268 6.782045242 7.823973377
H 20.152983887 7.657287663 7.875327085
C 19.160454752 6.044378209 6.742887858
H 19.376463142 6.164905412 5.693225767
C 18.272780956 5.080668975 8.597913441
C 21.149413834 5.000336171 11.513803754
H 21.827786109 5.813701974 11.710630459

C 21.336604303 3.661533586 11.672290891
H 22.176951181 3.100183202 12.049285440
C 19.258878018 3.996850375 10.804749668
C 17.008804476 7.317986046 11.900569351
H 17.443361383 8.257677194 12.200912496
C 15.793655586 6.779283565 12.188117148
H 14.970094393 7.151394432 12.776204894
C 16.916175838 5.319183634 10.866582336
C 19.815168978 7.903559435 10.876113315
C 19.632171567 9.055391041 10.085045286
H 19.047256609 8.992148849 9.172159698
C 20.153994876 10.298983319 10.447619619
H 19.993447132 11.160433497 9.803782462
C 20.869613696 10.438866002 11.636655767
H 21.281206033 11.403671890 11.921618486
C 21.030946093 9.328711253 12.465579246
H 21.561033718 9.426954125 13.409873748
C 20.503573987 8.090609107 12.091384036
H 20.614844741 7.257809849 12.779820934
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H 11.162608746 5.528824877 12.197051915
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⁵² (R=H)

Fe 17.638377111 3.835907223 9.830404010
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H 19.238577143 7.064759261 5.828059979
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H 21.956999035 6.229533600 11.342381330
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H 22.773647613 3.602450376 11.411078061
C 19.582737737 4.060439150 10.715874929
C 17.128220616 7.223096234 12.286375426
H 17.586547856 8.148803784 12.590809187
C 15.958630448 6.660126378 12.687220563
H 15.216631797 6.992525758 13.395952109
C 16.911182992 5.289555625 11.153048815
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N	20.676273190	3.282264090	10.925227898
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H	15.094052245	4.806691043	12.035932922
H	20.650319132	2.278310413	10.840410306
H	17.927595397	4.959304134	6.481980050
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C	14.977608373	1.669100278	11.516337376
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H	12.139665252	3.539947573	11.174274366
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H	11.719001227	2.622429505	13.450644561
H	17.020406423	0.120162389	9.078379730
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³²(R=H)

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C	19.145275806	5.433847646	7.075055566
H	19.515186728	5.185481101	6.092804230
C	17.648578270	5.529535541	8.782626524
C	20.195242465	4.805946212	12.132545725
H	21.168463460	5.267283449	12.139074188
C	19.798116553	3.622198603	12.669326350
H	20.336364795	2.885933412	13.245207072
C	18.014868965	4.558401553	11.619806464
C	17.500752382	8.730606721	11.504782028
H	18.327225094	9.410294393	11.631513731
C	16.175823337	8.912781662	11.737772507
H	15.626083841	9.765910910	12.101822771
C	16.477461812	6.794820219	10.973458872
C	20.244018149	7.730551967	10.800966747
C	20.605562124	8.625646222	9.774691225
H	20.081442976	8.590597494	8.823835077
C	21.608485237	9.582809802	9.940860844
H	21.860563758	10.248796518	9.119158909
C	22.278825230	9.690615008	11.159254602
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C	21.915369997	8.849128856	12.210534064
H	22.409216011	8.938063292	13.175078975
C	20.910344985	7.895979112	12.031374333
H	20.628985106	7.280955668	12.881219778
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N	15.566980437	7.706216187	11.402795923

H	14.579990007	7.512365895	11.463669923
H	17.865991834	2.704819036	12.553345092
H	17.197350128	4.548790789	7.005705343
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C	16.512328037	1.867722291	10.111238869
C	15.805754460	0.981070467	11.085732345
C	14.505722011	1.267052700	11.527239056
C	16.456785174	-0.147022849	11.607291463
C	13.871149436	0.438146577	12.451012650
C	15.824494824	-0.974564593	12.536411562
C	14.527060124	-0.685370033	12.961453257
H	14.014934560	2.156947499	11.143471055
H	17.468666391	-0.376797216	11.277971177
H	12.863561078	0.674537619	12.784086582
H	16.346617769	-1.842779374	12.930847015
H	14.033778759	-1.325333395	13.688068279
H	16.621760409	2.346120830	7.930793203
H	17.597249648	1.714073991	10.109991750
H	14.932862952	1.927159494	8.519703260

¹²(R=H)

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H	19.671653682	7.497570684	7.825395638
C	18.839956417	5.609258361	7.043924545
H	18.931406579	5.602117832	5.969369118
C	18.300691118	4.816923544	9.100666067
C	21.370952596	5.531368836	11.695795521
H	21.950422951	6.439267138	11.707129686
C	21.743006036	4.266089735	12.024585517
H	22.674760847	3.872027418	12.398385166
C	19.576062363	4.214327211	11.3171999884
C	16.965187562	7.329194764	12.153680915
H	17.257835268	8.361447738	12.259813706
C	15.876085995	6.672360093	12.632983583
H	15.046640953	7.012563327	13.232530391
C	17.135822860	5.192508078	11.455298069
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C	19.146576576	9.114860476	9.887516049
H	18.485287061	8.833149230	9.073305585
C	19.505766545	10.459245941	10.009264406
H	19.147104605	11.181702994	9.279922258
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H	20.600128179	11.920390265	11.164210011
C	20.729546871	9.937171130	12.011387042
H	21.335169082	10.249177915	12.858871723
C	20.363103309	8.595389941	11.877848644
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N	16.978628080	2.352378366	9.652450410
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C	12.769948141	2.212089720	12.722693606
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³¹P-TS (R=H)

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³¹P-TS (R=H)

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 O 12.115896012 -1.218785992 12.199358284
 O 11.221014836 -0.432254261 10.365335348

³1a (p-NO₂)

Fe 17.944983482 3.237623314 9.570894561
 B 18.694162700 6.230645676 10.431329443
 C 18.672408715 6.940207173 7.813150055
 H 19.014765409 7.952462273 7.948827834
 C 18.390465238 6.267621513 6.664241900
 H 18.411284686 6.581001364 5.632583396
 C 18.081047067 4.854460820 8.412906670
 C 21.175657397 5.374557173 11.102972856
 H 21.584389172 6.344091377 11.333762827
 C 21.783374468 4.155372253 11.103783487
 H 22.790120253 3.862335718 11.356220209
 C 19.632084319 3.883296932 10.435740670
 C 16.553632310 6.214041630 12.020733212
 H 16.707369076 7.211028513 12.399206205
 C 15.570364294 5.315335223 12.287056728
 H 14.708506799 5.371985157 12.932550234
 C 16.992226858 4.377257770 10.791543466
 C 18.948652907 7.733711623 10.967493280
 C 18.324339063 8.848736014 10.371533760
 H 17.693438063 8.3709963214 9.498489534
 C 18.455446499 10.140185660 10.887943444
 H 17.957895986 10.971780232 10.394959976

C 19.210154131 10.361421675 12.040409771
 H 19.316904702 11.364660060 12.444717036
 C 19.807187116 9.274497496 12.679369437
 H 20.372835738 9.424910869 13.595679022
 C 19.668436194 7.987827281 12.152883787
 H 20.111011132 7.161492438 12.701857955
 N 17.231370591 1.775965140 9.334592888
 N 18.458554553 6.074956909 8.876149735
 N 18.025511560 4.989417473 7.062514674
 N 19.857398635 5.192941913 10.718271902
 N 20.809888963 3.257824674 10.695751076
 N 17.418679206 5.629689320 11.102904624
 N 15.863548007 4.195657868 11.519283204
 H 15.312431219 3.350878637 11.472431774
 H 20.940673940 2.267563699 10.556583153
 H 17.781363808 4.227229544 6.449200471
 C 16.376152938 0.595843180 9.435165541
 C 15.433204455 0.738658267 10.582732169
 C 14.197855856 1.416704976 10.551049532
 C 13.671216856 2.022560768 9.364122872
 C 13.414565511 1.542076149 11.746269833
 C 12.467601449 2.696276113 9.375208001
 C 12.210761702 2.216809912 11.757870387
 C 11.738049331 2.795482415 10.570168119
 H 14.245072225 1.975788925 8.445800630
 H 13.784640116 1.088028229 12.662103722
 H 12.073762564 3.164753334 8.481341311
 H 11.621063494 2.314452074 12.661423921
 H 15.839853938 0.450125136 8.484859944
 H 15.795865607 0.412500517 11.555961709
 H 17.008567630 -0.292153654 9.575397799
 N 10.482190339 3.522327033 10.582690172
 O 10.082223010 4.004469215 9.517141923
 O 9.881909101 3.620163251 11.659498828

¹1a (p-NO₂)

Fe 18.274669563 2.721065585 8.255064285
 B 18.132216792 5.274183555 10.179185304
 C 18.679554401 6.901369270 8.076276402
 H 18.739633625 7.821356021 8.633198783
 C 18.885289605 6.678242725 6.748809645
 H 19.126794186 7.353190676 5.942932286
 C 18.421766036 4.690087935 7.745522568
 C 20.463384524 4.443679752 11.279329909
 H 20.601718054 5.283201738 11.939700960
 C 21.279452270 3.380624927 11.047774889
 H 22.230195570 3.107005140 11.476834899
 C 19.458419935 3.187698776 9.709265627
 C 15.662973426 4.516653172 10.850946327
 H 15.494311745 5.332204608 11.535021070
 C 14.847440751 3.492311909 10.485408513
 H 13.842917515 3.239321840 10.784860225
 C 16.806328585 3.265808214 9.371873183
 C 17.932459964 6.487068141 11.224679225
 C 17.289287226 7.687524687 10.862190412
 H 16.952224737 7.830749249 9.839734708
 C 17.031219077 8.702399079 11.786687645
 H 16.536470543 9.614718389 11.462836043
 C 17.395574638 8.542081856 13.123398880
 H 17.199235694 9.329677526 13.846205554
 C 17.994175425 7.347895122 13.525084412
 H 18.257146170 7.194417820 14.568837461
 C 18.246536402 6.341123314 12.590859827
 H 18.675805058 5.409433473 12.947479131
 N 18.315240968 1.114050898 7.896604554
 N 18.377340957 5.686624477 8.668468160
 N 18.715402161 5.314229300 6.574096274
 N 19.340694167 4.304522920 10.474441444
 N 20.633961356 2.619087995 10.083884925

N	16.858507030	4.368015337	10.161425367
N	15.571246215	2.742040313	9.569733696
H	15.263337037	1.881709184	9.137301980
H	20.981978181	1.774394167	9.658130555
H	18.815684237	4.817506672	5.702078557
C	18.268493966	-0.314393247	8.175489234
C	17.621650210	-0.541282100	9.502916094
C	16.235637809	-0.625133551	9.734924865
C	15.265356578	-0.587852962	8.681095376
C	15.737150641	-0.733692550	11.072041802
C	13.910871886	-0.643685115	8.949686737
C	14.386751737	-0.794967158	11.343078382
C	13.471862842	-0.744731609	10.279294292
H	15.599362845	-0.493318388	7.653584928
H	16.449982400	-0.756125672	11.891305198
H	13.173226457	-0.606967302	8.157109615
H	14.011044455	-0.871832952	12.356052561
H	17.732562438	-0.831977122	7.365656068
H	18.265580967	-0.488628635	10.378279693
H	19.288369133	-0.72797858	8.176293295
N	12.049266037	-0.783550410	10.558440852
O	11.694118897	-0.869011621	11.739758515
O	11.269296542	-0.723803270	9.600555729

⁵¹a (p-NMe₂)

Fe	18.440228097	2.710948585	8.657918822
B	17.832031335	5.368199512	10.368233559
C	18.509998842	6.997203295	8.327766509
H	18.440320525	7.912682695	8.890333736
C	18.902659199	6.805572855	7.039700979
H	19.206834178	7.505540173	6.277293577
C	18.435770290	4.777266771	7.952426371
C	20.105334975	5.032785494	11.759922017
H	20.040293360	5.967642582	12.290154256
C	21.089464320	4.096016749	11.779620729
H	22.011600355	4.043235945	12.336527776
C	19.491176884	3.421954464	10.309259878
C	15.395883450	4.466844902	10.920827925
H	15.117864172	5.341653198	11.484552647
C	14.684852675	3.343096569	10.645914445
H	13.684915940	3.049473745	10.923418266
C	16.722524057	3.136910703	9.680078353
C	17.377258812	6.619737967	11.294506763
C	16.647738449	7.705749766	10.769583823
H	16.426563840	7.740431749	9.707011816
C	16.162217451	8.737890746	11.575589196
H	15.609713957	9.559378669	11.125862063
C	16.374180782	8.709772476	12.953764941
H	16.001386332	9.512070037	13.585251393
C	17.050833291	7.625879284	13.512802062
H	17.197831990	7.571671364	14.588802612
C	17.530319393	6.600198328	12.695249649
H	18.014404799	5.751960115	13.170192551
N	18.715698327	1.384232073	7.534712961
N	18.200622239	5.755119314	8.870302092
N	18.841328852	5.435393505	6.838694702
N	19.117167502	4.600113681	10.882273306
N	20.683317804	3.117247718	10.884184409
N	16.648551970	4.332443583	10.327204688
N	15.522677420	2.545081687	9.880616211
H	15.293330318	1.632971023	9.504065863
H	21.209701070	2.294102937	10.636875291
H	19.090553251	4.951838122	5.989510284
C	18.615412653	-0.053709930	7.540510639
C	18.031382344	-0.657417534	8.793759807
C	16.649635981	-0.784067016	9.059869679
C	15.631821963	-0.382874780	8.143163470
C	16.178631983	-1.316966588	10.296647720
C	14.280757542	-0.513733383	8.432948832

C	14.835355242	-1.454422052	10.589298029
C	13.833331884	-1.070722647	9.658848974
H	15.918791777	0.060048091	7.194568876
H	16.910744914	-1.620041661	11.041212638
H	13.562069683	-0.180332541	7.692953215
H	14.554145722	-1.860711820	11.554043454
H	18.045407519	-0.389673900	6.654931319
H	18.720812329	-0.924240969	9.593419699
H	19.630752625	-0.458049903	7.381308877
N	12.481833490	-1.241342827	9.931915078
C	12.065389384	-1.610709079	11.280264922
H	10.975171694	-1.715921580	11.291923129
H	12.498751315	-2.584717757	11.578470037
H	12.354079471	-0.862041985	12.051959413
C	11.493368358	-0.643622054	9.042195981
H	11.594015431	-1.036875238	8.013103419
H	10.494117763	-0.908824500	9.401811351
H	11.562519026	0.465744721	8.987286078

³¹a (p-NMe₂)

Fe	18.262480687	2.768135682	9.810643513
B	18.315734064	5.908956136	10.487756300
C	17.363442028	6.364990551	7.993488399
H	17.384296897	7.440909125	8.042655562
C	17.049394878	5.553330981	6.948317612
H	16.730279066	5.778947133	5.943033714
C	17.640353477	4.251285712	8.713893963
C	21.018445647	5.924753248	10.364524805
H	21.143918462	6.986782871	10.494566768
C	21.956456115	4.963624946	10.141830933
H	23.031190092	5.021586314	10.070091656
C	19.905169938	3.976475020	10.136145558
C	16.914095077	5.347854156	12.690658238
H	16.856113737	6.366810880	13.035998537
C	16.424000788	4.204722097	13.237598436
H	15.856434393	4.034143912	14.138400025
C	17.496533248	3.663664761	11.316305036
C	18.197578802	7.460861493	10.930743602
C	17.078487340	8.237453909	10.566806557
H	16.306502554	7.803317464	9.938154690
C	16.902624808	9.548946956	11.012901833
H	16.025903151	10.112515958	10.702145764
C	17.842177350	10.131333639	11.863484201
H	17.711276493	11.152595717	12.212251685
C	18.939517049	9.376787678	12.278244742
H	19.665907639	9.805548986	12.964394126
C	19.103661478	8.065700369	11.824077243
H	19.948930770	7.497316749	12.201064622
N	17.523112030	1.324101055	9.572587765
N	17.700954843	5.561486165	9.074095432
N	17.223418226	4.259164895	7.419037806
N	19.777238360	5.310779297	10.382953617
N	21.245476853	3.780857477	10.011360394
N	17.567894101	5.004411643	11.514283928
N	16.807193688	3.182151226	12.380258120
H	16.514862906	2.216692555	12.422292738
H	21.644676922	2.874696590	9.820752951
H	17.109687703	3.410181226	6.887134332
C	16.366591594	0.436913565	9.544084380
C	15.288599700	0.743831060	10.549809529
C	14.355855814	1.801792684	10.444683122
C	14.360530010	2.737520033	9.371138639
C	13.355979783	2.015926309	11.437561897
C	13.468719331	3.791416729	9.304656317
C	12.459714547	3.067188776	11.376238024
C	12.484733142	3.995217481	10.303565460
H	15.117150930	2.646005796	8.601406514
H	13.303067426	1.331259739	12.282117730
H	13.551230326	4.480689333	8.472518957

H	11.734411321	3.174437207	12.174197367
H	15.941552462	0.454316638	8.523816148
H	15.210951354	0.092086367	11.419779865
H	16.715640117	-0.595490584	9.700165200
N	11.580905538	5.053591349	10.229529721
C	11.825888854	6.120964131	9.273779727
H	11.005384826	6.839924353	9.324475560
H	12.769773550	6.659864461	9.458260653
H	11.854793909	5.730178131	8.251265191
C	10.795377925	5.390174943	11.404822985
H	10.167556662	4.546490633	11.709391280
H	11.414467790	5.683569910	12.268107122
H	10.128891573	6.220749154	11.163244534

¹a (p-NMe₂)

Fe	18.558338922	3.000121773	8.335409177
B	17.799318596	5.382756446	10.357520486
C	18.525336040	7.208418146	8.487446315
H	18.392709718	8.084450468	9.100054295
C	18.986217748	7.108293804	7.210139781
H	19.298267665	7.862929336	6.505437003
C	18.556863999	5.013494926	7.983113969
C	19.974167771	4.699170624	11.827376020
H	19.901766941	5.495121955	12.549430716
C	20.920315838	3.730313147	11.699812226
H	21.795620322	3.509327328	12.289766446
C	19.416121862	3.484757016	10.016784893
C	15.373645454	4.300651142	10.579102334
H	14.996613515	5.049467690	11.256408779
C	14.771972055	3.197134611	10.062396969
H	13.781416772	2.794369928	10.200610188
C	16.882893791	3.292666818	9.243014600
C	17.284332617	6.492506833	11.416634654
C	16.592740120	7.652345573	11.012611652
H	16.430775174	7.841353879	9.955495406
C	16.068755325	8.566792178	11.929730125
H	15.545959548	9.450300193	11.571207328
C	16.204341038	8.343290061	13.300046369
H	15.801205418	9.052896964	14.017787415
C	16.844701409	7.182523315	13.734594860
H	16.934055636	6.975587788	14.798388293
C	17.363242292	6.276018480	12.807172012
H	17.818869021	5.364671497	13.183058752
N	18.732418633	1.463103497	7.787707565
N	18.245011935	5.929378694	8.939259023
N	18.989240652	5.751941288	6.926018724
N	19.045933982	4.526978661	10.809615186
N	20.550357467	2.994852279	10.582772395
N	16.665331264	4.348674216	10.072062515
N	15.716418056	2.600435279	9.240127926
H	15.602548898	1.712855840	8.768224646
H	21.044948685	2.208084337	10.192441283
H	19.295690845	5.331673593	6.062056368
C	18.571355113	0.017606177	7.779147216
C	17.976344941	-0.499580130	9.055116271
C	16.602677954	-0.718466584	9.301852612
C	15.583230972	-0.607490579	8.308311002
C	16.144122530	-1.059323098	10.610143320
C	14.239539632	-0.793245305	8.602537360
C	14.810208750	-1.254905207	10.905804392
C	13.805925273	-1.122504638	9.910794427
H	15.859373635	-0.358558006	7.287629112
H	16.879471048	-1.162167551	11.404906857
H	13.516614624	-0.676118620	7.802962084
H	14.534605404	-1.519790606	11.920802790
H	17.959349437	-0.270818896	6.910540047
H	18.647361090	-0.559407675	9.910144063
H	19.557708173	-0.449155790	7.615753229
N	12.465293156	-1.317327783	10.216358527

C	12.045585168	-1.327215487	11.609350686
H	10.936039248	-1.232199217	11.655125685
H	12.341321337	-2.273794257	12.133716551
H	12.487962432	-0.466019979	12.167030713
C	11.458740535	-1.165466911	9.178035568
H	11.703317538	-1.785852286	8.306902895
H	10.490018267	-1.502571592	9.557476105
H	11.347771947	-0.121249172	8.829509165

⁵1-TS (p-NO₂)

Fe	17.209104914	3.828253522	10.411771336
B	19.319568227	5.512292434	12.111919826
C	21.101116852	5.365706779	10.097969059
H	21.909769146	5.823315747	10.642366060
C	21.098958363	4.816264429	8.852647645
H	21.878573071	4.729182036	8.112491681
C	19.030461355	4.582691527	9.738235405
C	19.921309545	3.362381395	13.616336823
H	20.740553575	3.822428057	14.142442066
C	19.472497218	2.078601547	13.669123802
H	19.799814532	1.235261691	14.256452637
C	18.212526503	3.209831258	12.166436754
C	17.545945825	7.397014573	12.618607309
H	18.236874598	7.972283908	13.210656881
C	16.249049091	7.647205594	12.302683890
H	15.594402057	8.466057561	12.554835182
C	16.837660682	5.679431136	11.338400118
C	20.305301305	6.472545475	12.968371991
C	20.994480895	7.543331056	12.363383101
H	20.911078758	7.698172578	11.291306986
C	21.765669858	8.446132925	13.099291061
H	22.282007481	9.255263668	12.588584279
C	21.862510291	8.319455832	14.485430488
H	22.462129074	9.018331787	15.062689625
C	21.158027307	7.296861870	15.121340210
H	21.196239984	7.201123336	16.203751846
C	20.389680287	6.400592006	14.373356320
H	19.821708395	5.645195306	14.908668313
N	17.100636166	2.415812556	9.513108259
N	19.821587391	5.240816647	10.625223022
N	19.810506835	4.398027829	8.658806938
N	19.126446760	4.056562430	12.711627314
N	18.420097853	2.018536492	12.770959138
N	17.901478212	6.191284843	12.023227468
N	15.841808983	6.582467425	11.520389593
H	14.914620159	6.521922726	11.116518992
H	17.905362010	1.191326602	12.508182261
H	19.483051569	3.806295056	7.873456774
C	15.870240681	1.763037896	7.847432198
C	14.626870652	1.801911527	8.419541549
C	13.943093401	3.013260038	8.783962536
C	14.496491613	4.298387489	8.535687123
C	12.723368453	2.958926184	9.508220256
C	13.906685176	5.444986818	9.039498605
C	12.117955796	4.098358443	10.005491998
C	12.737790125	5.338753416	9.800575304
H	15.401399575	4.392803662	7.946678706
H	12.275188890	1.988337961	9.703792582
H	14.342435287	6.420875304	8.859544790
H	11.202368789	4.052166871	10.583773106
H	16.352615915	0.809881363	7.664275941
H	14.198945132	0.875669821	8.796231928
N	12.209829202	6.517133899	10.446482220
O	11.037305833	6.517588182	10.821110826
O	12.991049833	7.474324987	10.617806810
H	16.277594485	2.600566758	7.297058559

³1-TS (p-NO₂)

Fe	17.438914143	3.353650846	7.450407427	C	20.399716788	2.419987511	11.074005099
B	18.046348111	6.425354090	7.914113047	C	17.802207080	5.060298268	13.169293952
C	18.145050188	6.886103012	5.250878636	H	18.151500518	5.989458109	13.588683434
H	18.441909578	7.919070442	5.321068600	C	16.715977200	4.309630064	13.485869079
C	17.961801688	6.110914124	4.147557992	H	15.940285808	4.454971167	14.220445980
H	18.041344724	6.339030883	3.096420881	C	17.817313678	3.278733212	11.805268542
C	17.591047325	4.832814359	5.987524352	C	20.267904698	6.294979821	11.939386351
C	20.526865762	5.736427118	8.747851301	C	19.722948216	7.507567389	11.469659867
H	20.895376131	6.740964433	8.869483529	H	18.985944388	7.492974836	10.672118942
C	21.174357544	4.551082677	8.904053786	C	20.069349808	8.743442841	12.019659236
H	22.184571596	4.326874913	9.207090835	H	19.626681712	9.653959053	11.623340718
C	19.056169542	4.122203551	8.232084340	C	20.969465375	8.809081702	13.083115061
C	15.825719486	6.568054817	9.377806268	H	21.244631457	9.768602631	13.513283661
H	15.933497547	7.617605528	9.595659906	C	21.491712035	7.625123133	13.603304870
C	14.858654241	5.688240420	9.747482221	H	22.169888047	7.656514355	14.452546343
H	13.972134306	5.812900140	10.348153427	C	21.136383419	6.394910642	13.044675292
C	16.368758605	4.579593338	8.489737749	H	21.529828562	5.493741160	13.505289223
C	18.237726039	7.985824891	8.289698829	N	17.670519424	1.019110536	9.979423717
C	17.595809920	9.009209272	7.562778226	N	19.376725398	4.869926345	9.822345189
H	16.993481603	8.757934752	6.694550031	N	18.736930491	3.960197266	7.963587108
C	17.672653266	6.351917102	7.940206453	N	20.797353189	3.671326084	11.452858896
H	17.164088871	11.109183837	7.348683455	N	21.512058868	1.648426818	11.164610683
C	18.387312180	10.719976260	9.080022142	N	18.474698767	4.421945743	12.131108619
H	18.451374240	11.763527062	9.377067695	N	16.749981136	3.210816212	12.632918461
C	18.997267578	9.728105565	9.847589125	H	16.053359390	2.484456887	12.566255954
H	19.531253529	9.994151214	10.756527495	H	21.517693362	0.665865143	10.941335458
C	18.912220196	8.388925290	9.460033644	H	18.401570430	3.271019911	7.310062498
H	19.361624333	7.641929585	10.107622251	C	16.355839380	0.467697653	8.799265660
N	17.160970832	1.878052720	7.880790613	C	15.214342330	0.544872656	9.594917528
N	17.893920568	6.103137964	6.367081277	C	14.526885924	1.764642638	9.906562500
N	17.618581026	4.857985771	4.630721872	C	14.908637209	3.023775517	9.367100416
N	19.220769810	5.463955774	8.361202508	C	13.445464178	1.754134746	10.829115805
N	20.243420142	3.572917678	8.584994523	C	14.255299304	4.190568031	9.725504393
N	16.751579337	5.876429865	8.604499601	C	12.785914823	2.915332153	11.192611252
N	15.215665279	4.472571885	9.184129195	C	13.197494528	4.133502697	10.637944263
H	14.715749651	3.599482017	9.300945967	H	15.745355746	3.086015105	8.682259798
H	20.401753478	2.577366319	8.585702529	H	13.133793564	0.805506156	11.258475295
H	17.426934048	4.046616954	4.063183537	H	14.553580841	5.152027060	9.325415734
C	16.677816247	0.426765511	9.310201292	H	11.963717243	2.907740467	11.897813425
C	16.248408967	1.000397953	10.488931868	H	16.517831861	1.206107930	8.021172644
C	14.920714319	1.478924845	10.755388678	H	14.929446971	-0.335270604	10.166050958
C	13.869437983	1.442715020	9.792907700	N	12.524039893	5.361586095	11.030724289
C	14.615421616	2.061868490	12.015996998	O	11.616237083	5.281484616	11.865645196
C	12.613766405	1.958177004	10.070379786	O	12.898140460	6.418636909	10.511817830
C	13.364915668	2.576908066	12.302328354	H	16.739732860	-0.516902852	8.550584041
C	12.362337405	2.531126433	11.323867804	*****			
H	14.056783538	1.016950136	8.812415581	¹¹-TS (OSS) (p-NO₂)			
H	15.396408718	2.108773877	12.770187586	*****			
H	11.819407450	1.938888161	9.333663907	Fe	18.603416231	2.125136299	10.464117047
H	13.141685277	3.025902345	13.262530246	B	19.752627171	4.826489273	11.353441541
H	15.973070864	0.008284952	8.600456876	C	19.606612930	5.679073759	8.783044450
H	16.989902478	1.204771152	11.258864299	H	20.038917473	6.651086533	8.950575687
N	11.059698901	3.099978264	11.603206417	C	19.223507305	5.094254291	7.619558513
O	10.206544979	3.065641166	10.707107402	H	19.233235068	5.455836968	6.603751248
O	10.870115293	3.596479216	12.720536693	C	18.856883784	3.625424972	9.309070106
H	17.673292375	-0.000654963	9.261722916	C	22.186551846	3.708534638	11.729194992

¹¹-TS (CSS) (p -NO₂)

Fe	18.548970665	2.219973143	10.432647795
B	19.767601392	4.874147005	11.355850693
C	19.646345593	5.771332439	8.797405840
H	20.108277677	6.727582500	8.976495296
C	19.239584120	5.214486990	7.628368263
H	19.253571528	5.590116725	6.617733788
C	18.840472363	3.732159699	9.299417567
C	22.161282725	3.662928003	11.724558729
H	22.700537034	4.553066654	12.001070151
C	22.617649312	2.395176337	11.556504390
H	23.600980052	1.970329714	11.680939365

¹¹-TS (OSS) (p -NO₂)

Fe	18.603416231	2.125136299	10.464117047
B	19.752627171	4.826489273	11.353441541
C	19.606612930	5.679073759	8.783044450
H	20.038917473	6.651086533	8.950575687
C	19.223507305	5.094254291	7.619558513
H	19.233235068	5.455836968	6.603751248
C	18.856883784	3.625424972	9.309070106
C	22.186551846	3.708534638	11.729194992
H	22.694950139	4.621531750	11.988597745
C	22.687433613	2.456116047	11.574835878
H	23.686325087	2.068934759	11.697925161
C	20.466186353	2.393356331	11.107124075
C	17.803133226	4.983822138	13.183418086
H	18.127892674	5.931864361	13.579384025
C	16.744179391	4.207035748	13.529343096
H	15.973356655	4.344249061	14.270514182
C	17.857186416	3.175657663	11.855530464
C	20.199114861	6.279535284	11.901443141
C	19.586790148	7.452712055	11.413968371
H	18.839508907	7.382620555	10.628980326
C	19.878931998	8.716838790	11.929627196
H	19.384229842	9.594368557	11.520597894

C	20.791896871	8.852105453	12.975357020
H	21.025256916	9.834030396	13.378825849
C	21.381622009	7.708104141	13.512364738
H	22.071513061	7.793487609	14.348277308
C	21.079462710	6.448525192	12.988349707
H	21.524967967	5.579466309	13.462893195
N	17.756664520	0.932795511	9.933324297
N	19.355520098	4.785498417	9.819800061
N	18.754581476	3.831267544	7.969869929
N	20.821659069	3.663347364	11.466369481
N	21.606906237	1.665146118	11.200887780
N	18.481115980	4.345565143	12.149898533
N	16.803002148	3.092967608	12.699322613
H	16.133257480	2.340138649	12.663780726
H	21.647296928	0.680752754	10.989218870
H	18.455457877	3.116383981	7.326046433
C	16.294941151	0.574884100	8.692731807
C	15.152311300	0.668289361	9.473676347
C	14.502640609	1.896658421	9.847149767
C	14.944069585	3.171521925	9.402374842
C	13.388479285	1.864750475	10.727159225
C	14.312939091	4.335523480	9.808331753
C	12.750963288	3.022530275	11.139319524
C	13.219336777	4.256925858	10.675928639
H	15.808372491	3.247042197	8.753500896
H	13.031320641	0.902352818	11.084534969
H	14.654632298	5.309158562	9.478416768
H	11.902517451	2.998275545	11.812127725
H	16.546592014	1.373068940	8.002890622
H	14.797396578	-0.233952795	9.967299464
N	12.566129885	5.481068919	11.116645078
O	11.623459633	5.379768080	11.909083593
O	12.991420259	6.554630103	10.677407749
H	16.637687805	-0.407802658	8.386656538

⁵¹Ts (p-NMe₂)

Fe	17.402209138	3.741870104	10.202554128
B	19.154101047	6.100616398	11.517852993
C	20.785405883	6.178760024	9.382655794
H	21.472437522	6.893283859	9.803481067
C	20.858896086	5.502374755	8.204151895
H	21.589777975	5.532906857	7.411462525
C	18.984274789	4.835877836	9.291850770
C	20.398581439	4.398430606	13.186794623
H	21.091241642	5.121907710	13.582362342
C	20.319775690	3.061015493	13.423807829
H	20.898270495	2.418752306	14.069120756
C	18.715987299	3.611139917	11.914993848
C	16.967854852	7.516684864	12.011465112
H	17.513052752	8.323536733	12.471291844
C	15.630786315	7.372829678	11.811601592
H	14.801051225	8.016068356	12.058650939
C	16.667257547	5.536685539	10.984531172
C	19.893282737	7.382586060	12.182280278
C	20.243758966	8.511383045	11.414522004
H	20.070965855	8.505467982	10.342195026
C	20.782274687	9.665657107	11.987262072
H	21.042318577	10.511125947	11.354940064
C	20.974059310	9.739572657	13.366799845
H	21.394885191	10.634676127	13.817486159
C	20.597052937	8.657430851	14.161766613
H	20.711523182	8.709245164	15.241763912
C	20.059511286	7.508967525	13.575889894
H	19.738670720	6.703806503	14.230269602
N	17.176055124	2.249667077	9.432938916
N	19.620835026	5.784761286	10.031792001
N	19.736426043	4.691525367	8.175845993
N	19.396739361	4.732318855	12.282219395
N	19.275223123	2.609382585	12.633501272

N	17.599181017	6.386790348	11.500883261
N	15.477985976	6.150421933	11.180377583
H	14.600072222	5.748078675	10.873242178
H	18.978217108	1.650718738	12.531203088
H	19.507197857	4.014872336	7.463549578
C	15.383904198	1.325025015	8.693862348
C	14.488354393	1.526351876	9.707604007
C	13.697504808	2.722996834	9.940172962
C	13.655736177	3.826561007	9.061728632
C	12.909562306	2.835121329	11.105310132
C	12.871961239	4.948627066	9.318123590
C	12.128949956	3.949886489	11.380058219
C	12.086828888	5.049584757	10.491736343
H	14.241518615	3.806477530	8.147805617
H	12.909710464	2.012310253	11.816796658
H	12.871522627	5.751091905	8.589514515
H	11.543577578	3.958653546	12.291588723
H	15.864914449	0.361857364	8.580915639
H	14.431469392	0.773673463	10.492854943
N	11.328298707	6.192220920	10.769837653
C	10.365956733	6.135650087	11.858309301
H	9.575460695	5.382483868	11.704330035
H	10.865327631	5.910970220	12.806592651
H	9.891125387	7.113412180	11.964637758
C	11.022903538	7.102561058	9.676733337
H	10.420092272	7.928595980	10.059647321
H	11.937617445	7.535390919	9.257832693
H	10.468524057	6.621814044	8.854334006
H	15.416033791	1.966960908	7.821491606

³¹Ts (p-NMe₂)

Fe	17.641805183	3.387100392	7.714458866
B	18.611871018	6.301029376	8.564664645
C	18.345309479	7.183732837	6.018662307
H	18.747493612	8.168540856	6.187937126
C	17.921033445	6.610308718	4.859595244
H	17.860503167	6.997585725	3.854785652
C	17.718268821	5.082612563	6.528998586
C	21.110013978	5.306062965	8.888036690
H	21.589746858	6.245436624	9.105943025
C	21.652799678	4.065255763	8.763495235
H	22.667558713	3.718389005	8.876674945
C	19.428262596	3.914504901	8.350448041
C	16.689097925	6.315183911	10.408248212
H	16.923661123	7.300361731	10.776484145
C	15.733538411	5.432665147	10.801233548
H	14.982952662	5.487644705	11.573028887
C	16.894232615	4.492434415	9.106803243
C	18.997689850	7.768691753	9.132026375
C	18.346780517	8.933470242	8.675869623
H	17.597734799	8.859073274	7.892944671
C	18.602907575	10.194800007	9.219663152
H	18.079592042	11.065516205	8.831920878
C	19.516199659	10.336922389	10.264578524
H	19.720901445	11.316073282	10.689689959
C	20.143237751	9.198841118	10.771898661
H	20.833957116	9.284952592	11.607207817
C	19.878034868	7.943178456	10.219025805
H	20.354142222	7.077635135	10.669977767
N	17.161619980	1.901890739	7.888521940
N	18.195078499	6.251891346	7.034193116
N	17.537984775	5.323619805	5.204732652
N	19.744838438	5.201265891	8.659247049
N	20.595364455	3.228277307	8.437648672
N	17.398358810	5.728644696	9.365979778
N	15.880015943	4.323215327	9.982921603
H	15.335666353	3.470354576	10.038775440
H	20.651986717	2.236904773	8.263667856
H	17.188475101	4.624833600	4.567245530

C	16.438647056	0.289269491	8.929995964
C	16.114674389	0.623258286	10.230698432
C	14.886182173	1.251193905	10.670766499
C	13.826660633	1.613403914	9.803180734
C	14.703027411	1.594769925	12.030702161
C	12.687949329	2.270356351	10.256245717
C	13.570151673	2.249656989	12.494530331
C	12.517904117	2.606512976	11.619222178
H	13.911654578	1.403075033	8.741046527
H	15.491446385	1.352600627	12.739627535
H	11.927883088	2.533995658	9.530181886
H	13.512201779	2.492113829	13.549191645
H	15.662679054	0.164171176	8.181138114
H	16.887778629	0.522730665	10.991225791
N	11.367196420	3.255349636	12.078146996
C	11.376977426	3.819732683	13.416206667
H	11.554110128	3.042002348	14.166498276
H	12.141976215	4.603286008	13.555503409
H	10.399024138	4.257921870	13.626460284
C	10.496216469	3.893382017	11.105285354
H	9.646110651	4.339350357	11.625999491
H	10.998936003	4.684996479	10.524230304
H	10.095967178	3.159907339	10.397516352
H	17.336020903	-0.292593876	8.747483102

¹¹Ts (CSS) (p-NMe₂)

Fe	18.426083759	2.349510313	10.654322483
B	19.411155100	5.069675591	11.729764541
C	19.843983458	5.855709399	9.165099899
H	20.256856022	6.824129816	9.392952174
C	19.700373776	5.242651830	7.962393232
H	19.934198183	5.573152371	6.962731940
C	18.955941429	3.826573768	9.577517218
C	21.665658445	3.903768117	12.668056788
H	22.135422556	4.807741067	13.017823375
C	22.142486865	2.632553952	12.659375772
H	23.072706214	2.219335772	13.015994094
C	20.079675405	2.623066830	11.697045137
C	17.091254711	5.297613811	13.054419793
H	17.326876424	6.250094820	13.500759887
C	15.971563272	4.535570588	13.153914185
H	15.052930135	4.688975687	13.697310404
C	17.439005360	3.453835603	11.812928257
C	19.759110139	6.528344864	12.338666580
C	19.319088920	7.706707248	11.701525138
H	18.777934089	7.637667325	10.762435044
C	19.524697559	8.974441879	12.249787063
H	19.172929890	9.856224767	11.719089394
C	20.169220384	9.109345442	13.479403038
H	20.334736435	10.093870453	13.909769288
C	20.577610682	7.961868924	14.158918913
H	21.054803840	8.047592124	15.132236203
C	20.365683541	6.699381790	13.598832833
H	20.661140942	5.828408549	14.176103378
N	17.643096806	1.147108461	10.030928937
N	19.361817053	4.998524859	10.149210153
N	19.139269208	3.998930752	8.239049468
N	20.395052538	3.891924158	12.103755553
N	21.145703384	1.863717341	12.067665406
N	17.988528426	4.628759470	12.227723511
N	16.212301906	3.399928643	12.387279183
H	15.545244277	2.673349086	12.172093446
H	21.197654692	0.873657532	11.889057495
H	18.957142031	3.272048337	7.566261551
C	16.508642007	0.501184537	8.730762654
C	15.297973360	0.581622140	9.411583948
C	14.5444861394	1.789282768	9.623806183
C	14.897913371	3.038645631	9.058881524
C	13.423888499	1.792220881	10.485751504

C	14.195418241	4.197825531	9.341246151
C	12.710771810	2.946547229	10.776249996
C	13.077348351	4.192070212	10.210323635
H	15.765873836	3.108796488	8.413317802
H	13.117404974	0.856379329	10.948542932
H	14.533339592	5.125328996	8.895175355
H	11.870518649	2.879387361	11.456784993
H	16.733373074	1.220452212	7.949494490
H	14.988712291	-0.284325626	9.993973674
N	12.376034937	5.357099482	10.493176256
C	11.352502366	5.336509193	11.523094169
H	10.583284607	4.591462454	11.293322781
H	11.751081148	5.113967360	12.526863606
H	10.862675754	6.311398549	11.560221250
C	12.979686728	6.641103616	10.168329661
H	13.948637452	6.793156511	10.668310729
H	13.135038410	6.742888675	9.088681600
H	12.303885295	7.440579320	10.477059595
H	16.929227963	-0.484103844	8.553538164

¹¹Ts (OSS) (p-NMe₂)

Fe	18.466810470	2.277182751	10.687593358
B	19.357385993	5.036364579	11.719758613
C	19.753326696	5.805995123	9.146415783
H	20.127296712	6.792036163	9.365642016
C	19.632706808	5.177463183	7.949170830
H	19.852336325	5.508085199	6.946399808
C	18.945577365	3.748612140	9.575786147
C	21.662646895	3.977640395	12.661059263
H	22.100041714	4.906448543	12.986336855
C	22.189753694	2.726755366	12.673158590
H	23.138646556	2.358171820	13.029457684
C	20.122275201	2.615405748	11.730104971
C	17.047988816	5.207434609	13.067332949
H	17.258822664	6.174556551	13.493870744
C	15.954850186	4.411928954	13.196567490
H	15.038179111	4.546637332	13.748060403
C	17.437987959	3.353189367	11.855401588
C	19.650314141	6.520265620	12.295972179
C	19.135285456	7.660918710	11.646056988
H	18.578553081	7.543937252	10.720799824
C	19.287429037	8.948850649	12.163329807
H	18.877841693	9.799808043	11.623914512
C	19.953398335	9.142836227	13.373510630
H	20.078253955	10.143526759	13.779517185
C	20.436902784	8.032704639	14.065424848
H	20.932778654	8.163800224	15.024214728
C	20.276553261	6.749024144	13.536976135
H	20.628859222	5.907578647	14.125679649
N	17.755975727	1.049883869	10.038077230
N	19.305109199	4.939368485	10.138691114
N	19.121569452	3.915134788	8.237029240
N	20.388223525	3.903910887	12.108864816
N	21.219826491	1.907168956	12.105448617
N	17.954602325	4.553095316	12.238917673
N	16.222859227	3.270247527	12.448944942
H	15.574893881	2.521581458	12.253889541
H	21.310267763	0.916777826	11.944612864
H	18.972477933	3.172852921	7.572758075
C	16.484039042	0.514593163	8.693452919
C	15.256937096	0.626793275	9.332427089
C	14.554693126	1.861948808	9.579066750
C	14.993830152	3.120392775	9.102093407
C	13.394537600	1.875273120	10.386606705
C	14.333987413	4.296987912	9.417368440
C	12.724722807	3.047034858	10.710183256
C	13.176874745	4.300830320	10.233103309
H	15.893647471	3.182021973	8.499618772
H	13.020378283	0.932385834	10.780388366

H	14.736400393	5.228923083	9.038904718
H	11.850626093	2.985367904	11.347357919
H	16.788023507	1.266416601	7.972626307
H	14.872269510	-0.251534183	9.848661528
N	12.517738774	5.484246962	10.547875100
C	11.443562334	5.457654918	11.524326904
H	10.655696590	4.761871940	11.216983461
H	11.778848944	5.165520591	12.533660098
H	10.994839057	6.450869930	11.589567260
C	13.209403335	6.748930365	10.346931347
H	14.153532782	6.810326012	10.909768328
H	13.434531881	6.912537569	9.287405515
H	12.560856648	7.564648366	10.671417426
H	16.872869499	-0.478649787	8.492933471

³¹a-TS (p-NO₂)

Fe	17.408257703	3.839346308	9.809119542
B	18.882463175	6.453831148	10.651620559
C	19.286722810	7.059020406	8.044401366
H	19.852989454	7.957360517	8.221847881
C	18.984387422	6.446966406	6.869854097
H	19.208802224	6.713604957	5.849403146
C	18.130272881	5.201873111	8.561429781
C	20.987720445	4.975316267	11.511452173
H	21.632041333	5.802567162	11.756425503
C	21.239032117	3.640171437	11.560740313
H	22.111365497	3.090859204	11.877115949
C	19.136199995	3.941148838	10.767946536
C	16.758030958	7.148106549	12.111423494
H	17.171681765	8.093766150	12.419802773
C	15.565398429	6.573184146	12.415918199
H	14.746089593	6.912574040	13.029453214
C	16.689049687	5.172564272	11.043929074
C	19.507993201	7.852071992	11.161228411
C	19.227246016	9.067745167	10.505566177
H	18.617885900	9.066092054	9.606496523
C	19.677618975	10.296895632	10.991846170
H	19.441466887	11.210201431	10.451480139
C	20.416130629	10.354765709	12.173827282
H	20.770987116	11.308675718	12.554984118
C	20.670924676	9.175311167	12.873036228
H	21.216535882	9.206111413	13.812863144
C	20.214637041	7.952445171	12.376149247
H	20.392908489	7.062030958	12.971490963
N	16.301409972	2.783548878	9.075730739
N	18.740826784	6.304741507	9.077531187
N	18.266324375	5.309634875	7.217268140
N	19.689242282	5.150455599	11.051710381
N	20.080432996	3.025631817	11.104544274
N	17.445280611	6.278978532	11.269620565
N	15.549298256	5.356668213	11.747475494
H	14.785990977	4.693327902	11.747962913
H	19.946711141	2.032394590	10.995591995
H	17.902819067	4.622221453	6.576411294
C	15.230506104	2.094919376	8.443249723
C	14.513444374	1.973037066	9.741198671
C	13.587639450	2.916163131	10.253037213
C	13.122141019	4.046003307	9.511850443
C	13.065901696	2.757093787	11.574984376
C	12.202562472	4.930176318	10.039771187
C	12.146619828	3.640771772	12.108724167
C	11.712588186	4.732641749	11.340128383
H	13.511514219	4.228062542	8.516665677
H	13.400970926	1.910716282	12.169138842
H	11.854513811	5.787080389	9.475377301
H	11.753725682	3.515050580	13.110588660
H	14.701413071	2.677353830	7.675642881
H	14.829472590	1.161952163	10.388484527
H	15.524957611	1.128455333	8.009353198

N	10.765323760	5.669783221	11.899199900
O	10.383368885	5.486394697	13.063769336
O	10.386966624	6.609294642	11.187737394

¹a-TS (p-NO₂)

Fe	17.307541487	4.071821213	9.592034702
B	18.962107965	6.607534861	10.561541651
C	19.800945211	6.891374496	7.990111895
H	20.479915802	7.710781477	8.156537902
C	19.540098502	6.200694281	6.848470995
H	19.916984882	6.317175946	5.845081600
C	18.316449450	5.294657127	8.522908826
C	20.666635811	4.958659730	11.881663368
H	21.353885622	5.718639204	12.213285614
C	20.725552203	3.608002895	12.044050108
H	21.440436894	2.983130362	12.555828909
C	18.871864906	4.102971403	10.828527791
C	16.692440668	7.587460066	11.579517542
H	17.134672589	8.492486177	11.962469463
C	15.406756012	7.148458741	11.629121588
H	14.520204310	7.585343552	12.060677255
C	16.638540478	5.597012764	10.531712607
C	19.672496772	7.956619170	11.086374192
C	19.710349438	9.127182323	10.303002048
H	19.295932009	9.117077302	9.298917928
C	20.240830370	10.326487003	10.783119318
H	20.256499065	11.204671636	10.142271844
C	20.737782498	10.401805309	12.084512429
H	21.153331003	11.332335993	12.462171126
C	20.672594731	9.273894604	12.902705449
H	21.027184710	9.324288771	13.929455435
C	20.140384107	8.080377119	12.410284331
H	20.068657178	7.234598831	13.088137404
N	16.290476570	3.167460591	8.617270422
N	19.027018539	6.346270153	9.007011547
N	18.616224221	5.226372893	7.202089456
N	19.519408296	5.251149779	11.162506969
N	19.609847878	3.108345178	11.391008305
N	17.436996064	6.627494618	10.909675278
N	15.399783817	5.923412582	10.977351931
H	14.583583746	5.347227283	10.819353505
H	19.374033600	2.132484198	11.293882190
H	18.218594946	4.523137247	6.598776183
C	15.063612646	2.636993124	8.097607933
C	14.488488246	2.176305615	9.402949516
C	13.552646969	2.866318978	10.206226562
C	12.877174642	4.058242830	9.789562637
C	13.220419976	2.357859443	11.501438882
C	11.948467898	4.682094275	10.602845574
C	12.295501997	2.977142566	12.314712816
C	11.660621852	4.146491005	11.867444156
H	13.092891766	4.481848088	8.814622731
H	13.719069878	1.456875516	11.848034534
H	11.433825950	5.582051501	10.287130754
H	12.051308453	2.590221983	13.296724310
H	14.436816095	3.385340632	7.588034657
H	14.934392359	1.275481391	9.815060018
H	15.220145763	1.799229353	7.399546497
N	10.704808200	4.813395517	12.725715964
O	10.456870862	4.302320548	13.825256538
O	10.189899621	5.861386274	12.314390250

³¹a-TS (p-NMe₂)

Fe	17.466757282	3.717701699	9.914397389
B	18.995539175	6.262314521	10.875963231
C	19.664415636	6.847843866	8.318763785
H	20.254379824	7.718869231	8.548350527
C	19.442574819	6.249760862	7.119582007

H	19.772576602	6.505048796	6.125005686
C	18.378642223	5.042824501	8.724638085
C	20.935059695	4.683803381	11.920632516
H	21.600749731	5.476655605	12.215850026
C	21.108848561	3.338432087	11.998405891
H	21.920160969	2.747319030	12.392599893
C	19.098008169	3.742323132	11.020782000
C	16.794285951	7.087920668	12.137265363
H	17.228542724	8.016334584	12.469622795
C	15.553110281	6.577620793	12.347638062
H	14.706935697	6.965924347	12.891861379
C	16.712714350	5.097448186	11.087100614
C	19.645635608	7.634605693	11.436223589
C	19.469512032	8.858690024	10.759205641
H	18.932429865	8.876824766	9.815333605
C	19.933457144	10.070592561	11.275149593
H	19.777951140	10.990261600	10.716070361
C	20.582409200	10.103931358	12.509490644
H	20.948231150	11.044044856	12.914481380
C	20.735429738	8.917439999	13.226251593
H	21.213140128	8.929453521	14.203010605
C	20.264451832	7.712385837	12.699479794
H	20.361166749	6.817915460	13.307076405
N	16.400069428	2.656551758	9.092513669
N	18.991504644	6.120695198	9.295590798
N	18.642522017	5.147833560	7.397377651
N	19.691297715	4.924771726	11.350203481
N	19.961016210	2.782203966	11.447255738
N	17.502906702	6.172399578	11.366024001
N	15.529811300	5.353168731	11.693726212
H	14.735485250	4.729480897	11.634924524
H	19.784408581	1.797804667	11.323728715
H	18.311884261	4.473148149	6.726260443
C	15.327389865	2.006964777	8.418850365
C	14.520267422	1.947564818	9.663832642
C	13.621607971	2.966556732	10.107683145
C	13.252344617	4.091167193	9.324132584
C	13.037660989	2.903635970	11.399280049
C	12.375806383	5.059934265	9.786056453
C	12.156620612	3.869761993	11.869641924
C	11.788234888	4.980248278	11.072199231
H	13.692285930	4.223259673	8.341082131
H	13.296388807	2.071482985	12.050145087
H	12.157316311	5.901548787	9.139559879
H	11.758027917	3.758014387	12.871177460
H	14.874766291	2.596285218	7.606426508
H	14.759791476	1.146454271	10.355637125
H	15.590751878	1.015963518	8.018050046
N	10.892309699	5.948446886	11.529533340
C	10.545899598	5.967533505	12.940074923
H	10.083887433	5.021733821	13.242067297
H	11.412296409	6.145998189	13.599940827
H	9.814455434	6.758508475	13.117887244
C	10.803496460	7.210646476	10.813219595
H	10.051835378	7.840606204	11.293364377
H	11.756333231	7.765288710	10.791717823
H	10.482819735	7.051983859	9.778279896

¹a-TS (p-NMe₂)

Fe	17.514623951	3.765209385	9.710739718
B	19.380181221	6.296050414	10.154865760
C	20.054571035	6.120495448	7.531807419
H	20.782048756	6.914812856	7.525390308
C	19.692354278	5.272525878	6.533041876
H	20.015578605	5.203948597	5.506495952
C	18.521343016	4.717293887	8.398211868
C	21.087802254	4.761889031	11.605259233
H	21.844543225	5.512508219	11.761713002
C	21.080513071	3.452498426	11.976114226

H	21.797681414	2.865038781	12.527391909
C	19.162196773	3.882217166	10.828107344
C	17.255951774	7.573537290	11.162345133
H	17.776158165	8.495224016	11.367598734
C	15.955608245	7.233350247	11.368522640
H	15.131382498	7.791736578	11.783099492
C	17.011631357	5.449857268	10.448366633
C	20.201747793	7.663876208	10.407769078
C	20.239518738	8.693713006	9.446865010
H	19.741507616	8.554491679	8.491910135
C	20.875194779	9.913785095	9.687194738
H	20.886027357	10.678633629	8.914337835
C	21.485386532	10.155556058	10.917805856
H	21.984078049	11.102331817	11.108830565
C	21.427727921	9.174597158	11.907733754
H	21.872429949	9.358091175	12.882853590
C	20.789701779	7.958329052	11.653995368
H	20.729586766	7.233322880	12.460555728
N	16.366083624	2.840020110	8.872053570
N	19.315885168	5.793473122	8.662487544
N	18.741057317	4.426503718	7.088162751
N	19.904659930	5.020083052	10.931077264
N	19.885988904	2.938685703	11.493215785
N	17.891625193	6.475821650	10.601031587
N	15.830319172	5.924168225	10.924199330
H	14.968371143	5.396374195	10.881730204
H	19.586256888	1.979048569	11.568589076
H	18.279798662	3.656524406	6.630077433
C	15.163505309	2.509041430	8.178153644
C	14.420558459	2.230890502	9.443369180
C	13.585340952	3.148034115	10.149015448
C	13.148150586	4.392626443	9.624241306
C	13.119852878	2.837888555	11.455203446
C	12.327538166	5.252342254	10.343466257
C	12.298572213	3.685452873	12.177801500
C	11.869141748	4.926652998	11.643686881
H	13.475129957	4.700184219	8.635612211
H	13.431736899	1.900043424	11.908675025
H	12.041540482	6.191216801	9.883375846
H	11.996241716	3.385522130	13.174465756
H	14.737183801	3.330124030	7.580626398
H	14.654744846	1.289347934	9.929987448
H	15.250192862	1.624206077	7.526955978
N	11.034103963	5.780040199	12.359109481
C	10.820788471	5.536627249	13.776349497
H	10.373896965	4.549870053	13.943005943
H	11.748995538	5.592748541	14.369031557
H	10.122810749	6.280722336	14.165183345
C	10.812939369	7.127705344	11.865343062
H	10.117363936	7.643002379	12.530316151
H	11.738269293	7.725171725	11.808492672
H	10.362686127	7.111451362	10.866652286

⁵2 (p-NO₂)

Fe	17.597226649	3.892421154	9.826458467
B	19.099558591	6.614748560	10.606526347
C	19.456935716	7.278435180	8.026109737
H	20.061391643	8.144845298	8.233040676
C	19.122349377	6.727557001	6.828820671
H	19.350302534	7.027283172	5.818149997
C	18.228748954	5.448148169	8.480589096
C	21.352340062	5.315080197	11.250667603
H	21.935833920	6.206574350	11.404242985
C	21.741345120	4.014591469	11.294235385
H	22.695591905	3.563662974	11.516808747
C	19.533228285	4.081252315	10.740281129
C	17.119545510	7.320911282	12.228416408
H	17.597411307	8.237699114	12.529290323
C	15.926391908	6.797964176	12.611805302

H	15.178275728	7.160911711	13.298703373	C	20.463757128	8.106951741	12.313941258
C	16.875107984	5.375764200	11.119805031	H	20.694883137	7.212692380	12.885168152
C	19.727764868	8.029357460	11.091200712	N	16.658705722	2.221983985	9.674504468
C	19.392576225	9.242912979	10.457395790	N	18.896150298	6.494168238	9.041265768
H	18.743906452	9.233548946	9.586339938	N	18.393334263	5.614058095	7.138326949
C	19.839765710	10.479165057	10.928254080	N	20.018603359	5.325710428	10.937344437
H	19.561292664	11.389197261	10.402666850	N	20.654357118	3.266155052	10.951417442
C	20.629863776	10.548209104	12.075555725	N	17.709164593	6.383871170	11.324795804
H	20.983564285	11.507339704	12.444435366	N	15.838384275	5.490608026	11.928343038
C	20.938955627	9.370961586	12.756554481	H	15.081173269	4.820660556	11.985855557
H	21.526105469	9.408171563	13.670912988	H	20.622638894	2.262879520	10.860877580
C	20.485449366	8.141046577	12.274341388	H	18.010849201	4.972887594	6.460864045
H	20.710179274	7.251344121	12.855137158	C	16.172600763	0.936906434	9.290808107
N	16.636139648	2.244596377	9.696528382	C	16.200716270	1.342607476	10.738809195
N	18.885669142	6.506505914	9.030277031	C	14.972202234	1.702162496	11.513340420
N	18.363673125	5.610604104	7.139931930	C	14.033629312	2.620808571	11.053300501
N	19.995094640	5.349659385	10.941935494	C	14.732636687	1.160653200	12.783842079
N	20.604596599	3.282361251	10.982835432	C	12.914358216	2.993673806	11.774109601
N	17.697309231	6.443585981	11.312185608	C	13.613266486	1.507438273	13.534437807
N	15.802245899	5.605329773	11.913360573	C	12.674049807	2.444557145	13.052954185
H	15.023383072	4.964426710	11.970366078	H	14.209875145	3.071584357	10.053300501
H	20.561355893	2.278272856	10.907112955	H	15.438178427	0.441546149	13.196257976
H	17.971573436	4.966901959	6.470341697	H	12.229076017	3.724443705	11.357208535
C	16.205844560	0.950701132	9.297975074	H	13.456250470	1.028665224	14.495912799
C	16.217432573	1.339543643	10.755573061	H	16.880247177	0.171152078	8.946754490
C	14.963499012	1.629145020	11.505227377	H	16.962365774	0.852612868	11.358053807
C	13.983454791	2.487812615	10.970906913	H	15.196439199	0.874262072	8.795868797
C	14.749878094	1.082500440	12.781649300	N	11.538673254	2.785406791	13.798208972
C	12.827562464	2.786896095	11.681903683	C	11.579497115	2.814477485	15.252738998
C	13.601161204	1.373798431	13.509175533	H	10.841437096	2.133797333	15.699792368
C	12.650999630	2.227685770	12.950504051	H	12.568279333	2.532920306	15.616597117
H	14.163189911	2.927063620	9.994151635	H	11.371214275	3.827450358	15.628617024
H	15.502191781	0.426320620	13.212047917	C	10.518275521	3.623021563	13.202682838
H	12.063157441	3.442593193	11.281985343	H	9.611658646	3.571936915	13.813343899
H	13.429792615	0.963643556	14.496973954	H	10.810401650	4.685799978	13.123977205
H	16.941838735	0.208276311	8.964115065	H	10.263859483	3.264847587	12.200677117
H	16.990225903	0.870487353	11.375059787				
H	15.233161238	0.847515208	8.802709107				
N	11.446671957	2.555606739	13.714301847				
O	11.310739209	2.038815688	14.825344188				
O	10.637149562	3.334005109	13.204055264				

⁵² (p-NMe₂)

Fe	17.633296869	3.847636074	9.801049881
B	19.105599168	6.582720184	10.619875457
C	19.469299669	7.279998848	8.048387235
H	20.067015413	8.148168407	8.267408096
C	19.145976430	6.739630186	6.843241793
H	19.378112773	7.051702699	5.837167561
C	18.251499685	5.435513906	8.476611153
C	21.373739603	5.304034651	11.255715532
H	21.944528344	6.200667856	11.426771524
C	21.779515176	4.008104240	11.282226179
H	22.738295921	3.566571525	11.504429192
C	19.573745677	4.054129487	10.712817579
C	17.119910662	7.232463473	12.260644255
H	17.578978213	8.155188432	12.573192014
C	15.943015597	6.673822900	12.645486551
H	15.194547249	7.008049004	13.346579816
C	16.908408660	5.301143235	11.121712213
C	19.714764797	7.999871325	11.124980301
C	19.369879494	9.216905904	10.503015382
H	18.726393821	9.209382712	9.628073421
C	19.800530130	10.452886473	10.990170980
H	19.515231306	11.365654009	10.472676255
C	20.582675598	10.517825358	12.143137983
H	20.923622502	11.476777328	12.524614901
C	20.900446721	9.336346346	12.812778334
H	21.481624787	9.369849349	13.731120393

Table S5. Vibrational frequencies (cm⁻¹) of all optimized structures.

⁵1 (R=Bu)

32.73	33.27	33.53	41.62	43.24	56.35
61.98	63.39	80.13	81.04	94.78	116.09
127.90	141.20	144.55	150.57	167.65	174.91
179.41	194.38	206.38	208.29	239.09	242.52
245.39	246.42	252.53	256.94	261.47	267.77
282.66	288.39	298.15	299.48	304.19	320.96
322.45	333.41	338.66	339.83	342.68	347.45
355.75	364.90	376.64	379.32	386.54	399.39
415.12	418.07	427.23	458.22	461.51	462.89
498.63	505.53	514.50	523.10	594.69	599.10
602.97	633.92	644.35	647.91	656.80	664.70
692.45	708.57	710.14	726.58	729.58	732.68
738.08	752.97	804.41	822.82	827.65	830.12
830.40	834.87	838.85	846.74	850.37	886.01
892.37	932.24	937.26	937.38	941.00	945.67
946.15	954.20	974.26	983.09	983.94	997.99
1005.21	1009.06	1009.71	1014.24	1016.06	1035.28
1037.81	1041.14	1059.20	1059.89	1060.36	1060.71
1067.14	1069.53	1070.38	1110.41	1139.86	1140.45
1146.28	1172.34	1172.41	1179.80	1188.70	1194.28
1222.61	1223.18	1227.07	1235.70	1252.16	1254.53
1256.44	1259.45	1261.70	1262.18	1287.74	1301.06
1304.42	1308.50	1310.43	1318.54	1323.63	1363.51
1368.76	1370.51	1384.14	1413.58	1414.21	1414.31
1415.84	1416.26	1416.90	1430.41	1432.09	1444.52
1444.65	1444.90	1446.75	1472.15	1485.33	1485.98
1488.59	1497.32	1501.59	1502.64	1503.34	1508.71
1509.16	1511.79	1516.09	1517.48	1519.40	1526.31
1527.89	1533.74	1537.39	1539.35	1541.33	1600.03
1602.90	1606.47	1624.49	1655.18	3034.05	3035.13
3041.59	3042.03	3046.93	3047.88	3050.26	3050.62
3054.63	3109.62	3110.08	3114.17	3114.41	3120.00
3120.26	3120.34	3123.06	3124.46	3128.42	3129.62
3132.15	3133.01	3133.24	3133.44	3135.69	3137.92
3138.53	3169.71	3177.75	3191.08	3197.24	3202.88
3308.00	3308.17	3308.57	3328.54	3328.79	3328.92

³1 (R=Bu)

28.72	33.79	37.59	40.39	46.15	60.81
62.99	71.77	84.74	86.88	98.16	122.69
127.68	130.63	155.34	164.81	170.95	180.63
186.20	201.04	204.03	210.71	236.51	240.63
242.16	245.67	252.24	254.63	268.81	273.55
282.47	287.57	291.54	304.64	311.51	334.34
335.53	345.89	346.42	351.17	355.46	360.07
362.09	369.25	383.90	387.55	390.17	408.02
410.54	417.82	427.01	458.55	462.77	464.52
498.80	501.88	515.13	525.30	593.95	598.86
601.50	633.70	642.75	644.21	654.17	663.03
698.08	709.62	714.51	725.82	729.17	732.18
736.96	753.72	806.41	822.98	827.53	829.28
831.11	831.75	835.89	844.20	885.51	894.46
933.56	937.28	938.08	941.23	941.70	943.03
953.56	975.71	980.71	981.66	997.54	1005.14
1008.71	1009.81	1015.34	1016.16	1033.08	1037.92
1044.31	1056.50	1057.88	1060.56	1063.03	1064.66
1068.11	1068.91	1069.64	1109.81	1139.73	1140.74
1151.07	1175.30	1178.51	1182.73	1188.54	1199.07
1223.62	1225.15	1226.54	1238.58	1250.36	1252.64
1255.15	1260.11	1261.70	1262.01	1289.07	1299.68
1302.22	1303.58	1311.23	1317.93	1320.68	1365.22
1370.19	1370.39	1385.32	1411.75	1412.98	1415.01
1415.95	1416.27	1417.02	1430.58	1431.02	1444.29

1444.68	1444.90	1446.90	1472.27	1486.40	1487.19
1488.42	1498.12	1503.35	1506.30	1507.43	1507.85
1509.20	1512.15	1514.23	1515.91	1520.26	1524.85
1525.55	1534.78	1537.41	1539.91	1542.18	1599.87
1612.36	1615.21	1624.62	1655.31	3041.29	3042.31
3044.96	3045.86	3046.40	3047.96	3052.11	3052.47
3054.50	3111.39	3111.84	3115.28	3115.53	3118.24
3121.22	3122.18	3122.54	3123.95	3132.19	3132.89
3134.25	3135.88	3141.91	3146.88	3149.81	3154.93
3156.13	3170.08	3178.02	3190.94	3197.40	3203.60
3306.18	3311.61	3311.75	3327.72	3338.16	3339.30

¹1 (R=Bu)

35.67	40.26	41.29	46.30	59.64	61.28
64.04	65.88	86.78	91.94	103.61	129.58
147.94	151.10	165.37	184.63	187.60	190.07
194.33	204.72	205.20	210.56	240.27	245.42
246.97	251.74	255.52	264.45	274.15	280.30
293.22	299.71	308.25	328.76	333.11	347.52
348.48	349.75	352.29	353.55	357.64	359.52
371.91	373.66	390.31	391.83	398.59	412.61
416.56	417.51	427.83	457.52	464.47	464.72
500.09	508.21	527.80	538.04	594.80	599.86
603.61	631.35	634.85	635.31	644.12	662.92
693.53	706.43	710.46	717.72	728.83	730.29
738.26	754.99	799.50	819.55	826.53	827.02
829.11	829.66	831.32	839.03	887.21	896.98
936.22	936.92	937.17	942.47	943.26	944.63
955.38	979.01	981.58	982.19	999.16	1006.31
1008.79	1010.25	1015.71	1017.76	1036.42	1038.65
1041.43	1061.36	1061.99	1063.19	1067.27	1068.34
1069.26	1069.85	1109.41	1138.01	1139.85	1147.92
1173.61	1175.96	1176.56	1185.12	1189.49	1201.21
1220.42	1223.03	1227.84	1239.31	1257.85	1259.81
1260.27	1261.51	1261.69	1262.74	1276.56	1288.09
1300.25	1303.07	1307.99	1314.46	1317.23	1369.94
1379.66	1383.69	1400.84	1413.40	1415.33	1415.42
1416.51	1417.44	1417.64	1428.71	1429.55	1442.00
1445.16	1445.48	1448.00	1472.53	1488.01	1489.24
1489.34	1503.26	1506.29	1506.99	1508.47	1510.01
1510.40	1514.53	1514.94	1517.61	1523.21	1524.38
1525.46	1538.08	1538.99	1539.66	1543.28	1613.69
1614.51	1617.11	1624.17	1655.54	3041.79	3042.19
3042.84	3043.47	3043.69	3043.86	3049.80	3050.15
3051.06	3109.43	3109.71	3110.13	3112.58	3113.01
3113.39	3118.64	3118.81	3118.83	3128.34	3129.21
3129.38	3151.13	3153.25	3153.71	3156.23	3157.41
3159.65	3164.72	3173.08	3187.07	3194.23	3199.12
3305.43	3307.75	3308.33	3332.09	3332.54	3332.79

Styrene

36.90	206.11	234.09	413.35	441.53	455.76
560.47	633.84	655.26	713.85	789.54	798.99
854.62	924.27	928.00	971.69	996.54	1014.60
1032.64	1043.60	1062.58	1117.67	1187.22	1210.77
1234.26	1327.31	1361.29	1368.16	1462.21	1493.64
1541.04	1634.07	1661.77	1710.28	3155.31	3169.06
3172.28	3180.12	3190.05	3198.90	3207.78	3250.17

(Z)-prop-1-en-1-ylbenzene

55.14	126.57	167.11	228.48	295.66	412.66
422.22	469.51	527.13	632.11	669.41	710.56
723.09	788.20	823.20	860.97	933.08	943.67
976.96	997.43	1005.53	1013.78	1056.46	1064.05
1094.92	1115.57	1187.10	1210.48	1218.94	1285.76
1354.11	1364.27	1413.27	1450.21	1486.85	1499.90
1505.75	1539.38	1630.83	1660.17	1719.70	3028.10

3078.51 3130.09 3140.39 3159.08 3172.43 3180.46
3190.39 3202.89 3215.69

(p-NO₂C₆H₄)CH=CH₂

44.89 70.16 115.71 177.10 277.53 283.67
346.85 420.29 458.85 494.36 541.96 626.62
637.11 646.52 721.11 782.50 788.84 848.28
871.06 882.66 945.08 987.78 990.95 1029.27
1033.73 1052.85 1132.94 1137.38 1211.22 1235.26
1321.20 1351.85 1376.50 1396.52 1446.44 1473.44
1536.35 1611.44 1654.21 1666.04 1707.30 3156.52
3169.82 3192.89 3209.50 3245.54 3245.94 3253.88

(p-NMe₂C₆H₄)CH=CH₂

53.94 70.01 103.49 150.62 161.15 207.94
214.79 296.10 333.02 365.39 422.04 461.59
494.11 511.70 547.16 656.10 656.29 693.95
759.48 813.51 817.72 837.11 901.21 948.47
949.60 968.22 1021.00 1033.80 1055.48 1084.80
1137.81 1150.69 1164.79 1200.67 1220.45 1255.07
1272.07 1330.03 1364.42 1368.31 1384.21 1452.99
1464.35 1480.81 1496.38 1497.94 1504.44 1524.15
1540.52 1570.03 1605.23 1673.05 1704.43 2982.98
2990.95 3077.28 3082.22 3131.32 3136.94 3140.94
3162.08 3172.90 3188.34 3225.54 3227.42 3244.58

⁵1-TS (R=ⁱBu)

-390.66 15.72 26.57 31.69 38.31 41.66
43.07 44.39 45.94 47.27 56.55 62.26
64.08 66.84 81.73 82.87 97.50 117.39
119.58 129.89 143.48 146.26 158.36 170.72
173.95 178.31 205.21 207.98 208.59 217.13
232.06 245.28 248.04 249.38 256.34 264.71
269.84 271.28 279.40 291.30 299.17 304.65
306.14 330.76 333.73 337.48 339.02 343.17
345.79 347.94 354.67 355.89 361.17 371.99
377.30 383.85 405.71 407.83 412.44 419.10
428.78 450.18 458.36 461.72 463.34 497.66
501.87 504.17 512.58 523.58 559.38 594.41
599.00 601.96 627.59 632.25 635.71 645.40
649.22 653.71 660.23 691.67 693.35 706.90
712.47 720.23 729.45 730.41 732.88 738.36
752.81 790.35 794.47 806.12 823.18 828.17
830.52 831.31 836.80 839.52 847.26 850.75
886.53 886.89 908.96 935.28 935.83 937.01
941.39 946.30 946.62 948.41 955.06 964.65
977.13 982.75 983.23 984.41 988.39 1000.65
1005.52 1006.85 1009.01 1009.22 1009.67 1014.62
1031.08 1035.93 1042.20 1046.97 1058.72 1059.53
1060.52 1061.34 1062.02 1064.70 1070.50 1071.49
1110.25 1114.76 1139.24 1142.01 1148.99 1171.72
1173.90 1179.39 1184.38 1188.93 1191.39 1206.37
1221.44 1223.11 1226.41 1234.69 1234.72 1252.26
1255.65 1259.36 1260.42 1261.30 1261.62 1287.39
1297.01 1302.08 1305.23 1306.35 1309.43 1317.22
1319.45 1345.45 1363.66 1366.58 1369.27 1371.10
1379.54 1413.08 1413.71 1416.73 1416.87 1417.75
1418.73 1429.22 1431.51 1443.22 1445.52 1445.96
1447.61 1450.05 1471.97 1486.89 1487.72 1488.63
1489.94 1496.15 1501.79 1505.78 1506.27 1507.82
1509.99 1510.31 1517.00 1517.61 1519.57 1525.00
1526.38 1533.62 1534.32 1536.32 1539.49 1541.66
1590.21 1599.87 1603.05 1605.73 1624.47 1625.90
1650.87 1654.36 3034.03 3035.82 3039.66 3040.12
3044.47 3047.28 3048.51 3048.86 3053.66 3108.24
3108.80 3111.39 3111.80 3118.57 3118.84 3119.73
3122.17 3124.43 3128.23 3130.16 3130.68 3131.38

3131.77 3134.10 3135.27 3137.08 3146.76 3149.31
3162.77 3168.89 3172.02 3176.25 3180.95 3183.53
3189.01 3194.14 3196.75 3201.24 3206.73 3265.99
3305.63 3306.10 3311.55 3327.36 3328.26 3331.64

³1-TS (R=ⁱBu)

-602.60 13.24 27.97 33.89 39.60 41.80
44.39 46.99 48.70 53.75 63.83 64.62
73.83 74.94 83.32 85.98 98.68 120.52
122.48 134.31 147.95 158.98 171.56 175.03
183.79 194.61 206.90 209.47 216.90 240.30
244.81 247.00 251.47 254.19 257.63 263.11
269.57 286.31 290.38 293.09 297.52 301.48
311.90 332.29 335.16 337.85 344.21 350.28
352.76 356.36 360.51 365.58 369.78 381.19
386.46 391.13 407.63 412.78 415.37 418.00
426.64 456.15 461.67 463.91 467.66 495.31
501.16 511.74 513.08 522.10 546.33 562.08
595.09 599.15 603.52 633.10 635.53 643.61
644.22 655.01 663.43 700.56 701.30 710.15
712.84 727.39 728.41 731.51 734.92 737.98
756.86 790.55 797.52 810.10 827.07 828.69
830.90 833.20 834.46 836.84 846.00 847.91
886.33 896.41 903.84 936.51 936.98 937.17
941.47 942.31 942.76 944.41 954.28 962.08
978.07 980.09 980.92 984.44 998.34 1005.66
1006.44 1008.15 1010.16 1015.85 1017.31 1033.26
1037.21 1045.03 1052.12 1058.14 1059.47 1060.84
1063.95 1066.71 1067.80 1069.48 1069.82 1078.35
1110.19 1116.83 1139.32 1140.91 1150.33 1174.70
1177.06 1181.53 1184.04 1188.84 1198.20 1206.70
1224.07 1224.92 1226.97 1232.82 1238.06 1248.75
1253.66 1256.84 1260.85 1261.40 1263.23 1287.44
1290.51 1301.88 1304.68 1306.22 1311.84 1318.20
1321.91 1344.16 1363.05 1367.28 1369.95 1370.82
1385.48 1412.00 1414.26 1415.36 1416.20 1416.37
1418.92 1428.61 1430.66 1443.61 1444.32 1444.48
1446.14 1447.58 1472.63 1486.43 1487.85 1488.60
1488.67 1496.97 1501.80 1505.95 1507.12 1508.61
1509.53 1511.00 1513.54 1515.76 1519.95 1524.34
1525.12 1532.04 1534.28 1537.65 1539.75 1541.93
1567.57 1601.92 1611.90 1616.61 1620.11 1624.83
1648.86 1655.11 3040.33 3042.71 3043.98 3045.02
3045.91 3046.83 3050.74 3052.10 3053.17 3109.77
3111.52 3112.62 3115.12 3118.57 3120.83 3122.75
3123.29 3124.96 3130.91 3131.36 3134.69 3139.86
3145.08 3146.50 3148.03 3149.68 3155.35 3156.15
3159.85 3163.54 3167.85 3171.90 3175.74 3181.19
3188.76 3194.66 3196.66 3200.74 3205.05 3235.57
3307.67 3308.34 3310.66 3328.00 3332.68 3333.70

¹1-TS (CSS) (R=ⁱBu)

-798.6 24.02 36.31 38.39 39.08 47.84
49.15 49.75 51.47 59.79 60.89 64.76
70.72 79.50 83.61 117.08 120.58 143.53
144.85 161.89 176.22 209.68 211.35 216.97
218.35 223.19 230.88 232.60 233.28 235.00
235.29 236.77 239.26 244.64 246.98 247.22
254.18 259.65 280.26 282.94 312.76 325.37
336.12 348.89 356.73 359.97 360.69 373.21
377.15 383.29 386.47 394.67 395.20 410.62
411.45 423.57 431.71 442.35 448.55 456.95
484.15 489.11 511.10 533.87 542.75 544.80
547.72 565.77 595.95 607.38 617.04 625.95
644.85 656.28 677.74 693.65 699.20 730.27
749.06 757.67 764.49 786.25 789.40 790.47
821.10 852.12 858.40 861.21 898.84 904.33
913.50 924.52 936.01 936.19 937.49 937.85

962.88 981.59 985.98 990.08 994.69 997.14
 1006.59 1017.36 1020.83 1023.33 1023.93 1024.43
 1026.24 1026.45 1027.95 1034.35 1036.37 1037.25
 1055.71 1060.02 1061.38 1078.06 1104.24 1118.00
 1138.16 1172.15 1189.07 1190.61 1192.09 1199.04
 1205.96 1208.74 1233.22 1234.03 1237.18 1248.67
 1249.18 1258.38 1261.26 1270.21 1278.70 1279.72
 1282.26 1296.40 1306.31 1310.31 1312.27 1313.01
 1315.87 1333.53 1347.03 1354.66 1374.34 1393.45
 1396.47 1419.27 1465.73 1471.85 1478.62 1482.60
 1485.88 1487.06 1507.28 1524.19 1576.36 1580.77
 1585.96 1596.31 1606.73 1607.86 1609.13 1613.32
 1615.71 1618.92 1621.05 1621.73 1625.65 1626.18
 1626.68 1634.84 1635.99 1637.66 1646.89 1647.63
 1648.05 1654.38 1655.74 1655.87 1656.34 1656.67
 1656.67 1657.31 1657.79 1657.84 1657.99 1659.22
 1659.66 1660.23 1663.34 1665.74 1666.05 1666.79
 1683.82 1700.88 1705.48 1707.05 1716.85 1732.30
 1733.33 1734.60 1734.95 1747.67 1750.74 1775.59
 1776.67 1777.56 1789.29 1797.94 1832.24 1843.78
 1848.83 1868.38 3020.07 3020.39 3020.58 3021.33
 3021.45 3022.38 3022.49 3022.85 3024.29 3097.88
 3130.30 3130.70 3131.18 3132.84 3132.97 3134.56
 3135.45 3136.13 3136.18 3136.45 3137.02 3137.15
 3138.33 3138.73 3139.40 3143.59 3144.39 3145.79
 3146.86 3146.93 3147.66 3147.68 3148.23 3148.31
 3148.85 3152.45 3152.83 3154.79 3161.38 3195.36
 3195.96 3198.97 3199.91 3207.24 3207.60 3208.71

¹¹TS (OSS) (R=ⁱBu)

 -814.34 6.92 26.53 35.54 38.44 42.32
 46.71 49.37 52.59 54.75 63.59 69.04
 74.01 76.23 86.36 93.37 103.39 129.26
 141.33 150.24 151.63 166.90 181.95 187.02
 200.22 202.49 209.99 228.62 234.65 242.64
 248.67 255.09 257.31 263.24 267.25 268.41
 281.92 294.53 300.87 303.06 310.92 319.42
 334.90 347.24 348.98 350.07 350.50 354.51
 355.31 355.66 360.51 372.77 376.46 390.08
 395.79 403.08 415.90 418.07 419.41 422.38
 426.35 452.74 459.36 465.63 466.95 499.19
 503.81 506.68 523.99 533.40 556.69 592.60
 600.09 604.13 626.75 633.35 636.91 637.57
 638.97 645.86 666.50 693.74 698.27 704.48
 708.85 716.31 729.84 731.79 736.31 741.41
 755.25 783.33 806.40 807.81 821.93 825.49
 828.56 829.08 831.13 831.22 838.53 848.22
 885.46 898.39 912.79 936.25 936.62 938.04
 941.80 942.43 943.61 951.83 952.88 966.89
 977.15 979.17 981.77 989.61 997.44 1001.65
 1004.78 1008.58 1009.50 1015.96 1017.17 1038.05
 1040.04 1043.94 1050.15 1059.65 1060.42 1061.07
 1067.60 1068.97 1069.66 1070.10 1079.72 1109.42
 1115.40 1119.42 1137.81 1139.36 1150.23 1177.70
 1178.00 1182.83 1184.87 1188.76 1202.68 1205.24
 1223.65 1225.69 1227.50 1229.17 1240.97 1252.11
 1253.79 1255.92 1260.15 1261.03 1262.50 1280.82
 1286.35 1293.40 1300.55 1304.25 1308.87 1314.96
 1317.29 1345.27 1367.69 1368.96 1372.47 1375.15
 1391.86 1410.87 1412.55 1413.34 1414.40 1415.45
 1417.03 1427.75 1428.41 1441.79 1442.78 1443.28
 1446.28 1446.84 1472.82 1486.93 1488.16 1488.46
 1489.92 1504.48 1506.25 1506.90 1509.21 1510.03
 1510.29 1513.05 1513.35 1515.04 1523.18 1523.80
 1525.60 1530.41 1537.88 1538.78 1540.15 1543.25
 1559.84 1613.33 1614.83 1617.39 1620.62 1624.83
 1646.03 1655.46 3041.08 3041.92 3042.90 3044.61
 3045.59 3046.12 3051.63 3051.91 3052.66 3109.48
 3110.10 3110.54 3113.05 3113.85 3118.10 3120.02

3122.90 3123.15 3129.16 3130.00 3131.07 3149.08
 3150.15 3152.79 3153.55 3154.53 3157.48 3158.22
 3167.02 3167.09 3168.67 3175.37 3176.52 3186.38
 3188.95 3195.91 3201.25 3201.38 3214.48 3235.43
 3306.58 3308.28 3309.69 3333.30 3333.48 3334.81

⁵1a (R=ⁱBu)

 22.87 27.22 38.84 40.94 47.80 53.55
 56.88 59.51 62.40 66.25 68.77 75.80
 81.71 87.06 93.04 106.01 108.95 120.49
 135.68 144.91 146.65 158.21 167.90 179.44
 201.09 204.40 208.03 220.46 233.13 244.54
 245.99 249.75 250.92 257.84 260.12 265.55
 274.35 280.04 287.98 292.80 302.75 304.33
 315.35 336.49 338.54 339.23 341.05 346.27
 352.68 360.76 363.39 368.30 378.76 391.88
 403.97 408.72 414.05 421.01 421.31 429.63
 441.16 463.87 469.72 489.77 502.81 506.55
 508.80 519.48 524.67 573.45 597.24 598.87
 601.83 604.69 623.18 631.93 642.94 648.42
 654.29 657.51 663.88 695.23 699.73 706.94
 721.53 726.24 727.75 737.62 748.68 756.99
 784.08 812.38 827.07 828.74 829.91 833.95
 839.70 842.39 845.36 852.91 881.68 886.19
 894.30 933.75 934.33 934.66 941.93 942.94
 944.49 953.84 965.48 976.53 978.87 980.79
 981.88 988.19 989.14 1001.01 1003.78 1006.22
 1007.62 1013.99 1016.14 1029.20 1033.42 1039.46
 1045.30 1056.24 1059.58 1060.49 1063.42 1064.77
 1066.82 1067.96 1106.59 1112.28 1134.37 1135.48
 1141.35 1143.30 1149.54 1159.92 1171.44 1178.28
 1180.45 1185.94 1187.67 1192.36 1216.66 1221.01
 1226.37 1228.15 1235.19 1248.90 1254.35 1256.42
 1259.03 1259.98 1260.39 1278.56 1295.70 1297.51
 1302.59 1306.89 1309.75 1315.55 1320.87 1333.49
 1359.25 1359.86 1370.08 1371.09 1381.24 1402.21
 1410.48 1413.21 1414.40 1414.80 1416.80 1418.22
 1420.30 1424.58 1429.76 1442.20 1442.60 1445.36
 1446.67 1470.24 1487.72 1488.74 1488.96 1489.58
 1500.00 1502.13 1505.29 1506.07 1507.52 1508.72
 1512.19 1513.62 1514.88 1515.76 1520.82 1522.12
 1522.88 1535.65 1535.72 1537.15 1539.96 1585.19
 1594.03 1600.71 1609.24 1615.83 1622.73 1654.16
 2810.96 2865.87 3037.42 3037.91 3042.46 3042.70
 3044.62 3045.51 3048.46 3051.10 3051.54 3107.13
 3107.70 3112.81 3113.07 3115.16 3116.51 3117.76
 3120.92 3121.11 3126.75 3128.20 3130.45 3135.64
 3136.27 3139.25 3142.13 3145.16 3146.18 3150.50
 3152.75 3156.56 3167.09 3168.67 3169.68 3171.91
 3175.08 3184.80 3189.91 3194.50 3195.97 3201.90
 3301.57 3305.97 3306.96 3322.05 3322.22 3328.44

³1a (R=ⁱBu)

 10.69 30.48 31.58 33.93 39.51 41.64
 46.99 48.28 61.39 63.00 64.85 69.24
 70.30 81.10 85.29 97.57 105.19 118.96
 133.90 137.98 147.94 165.26 176.36 179.85
 192.59 204.17 206.69 209.10 222.11 237.60
 242.97 247.79 254.70 255.12 255.84 259.88
 283.80 285.75 295.17 296.63 305.05 317.60
 330.88 334.71 336.42 338.74 342.36 349.12
 353.33 356.58 361.09 372.37 375.04 381.29
 388.39 408.91 410.42 415.71 428.83 453.33
 459.35 460.00 463.95 479.49 494.90 500.85
 508.24 513.49 522.62 549.54 578.66 590.78
 598.33 622.73 631.23 637.92 642.93 644.42
 654.09 661.09 683.20 694.08 701.20 709.92
 720.96 725.69 727.83 736.42 750.10 761.87

774.75 787.75 815.86 826.23 828.51 830.21
 830.44 831.97 836.40 843.42 885.58 885.86
 886.68 904.10 934.37 934.70 935.58 941.11
 942.82 945.31 947.51 958.65 962.18 976.56
 979.49 980.77 981.67 986.41 999.96 1005.34
 1007.29 1007.67 1011.25 1028.58 1030.80 1035.51
 1040.40 1054.20 1058.20 1059.00 1064.18 1064.55
 1065.06 1067.13 1069.66 1083.84 1102.31 1110.25
 1120.97 1137.99 1145.98 1166.98 1170.47 1178.00
 1179.00 1187.56 1187.77 1193.76 1199.08 1209.32
 1221.79 1225.97 1229.10 1235.20 1251.52 1252.14
 1253.68 1259.55 1260.75 1261.54 1270.62 1289.42
 1302.48 1304.22 1305.39 1314.95 1317.03 1318.71
 1339.79 1354.50 1362.40 1366.12 1369.92 1374.98
 1399.59 1411.49 1413.67 1415.07 1415.60 1416.22
 1418.09 1427.58 1437.10 1438.04 1443.17 1444.18
 1444.63 1446.19 1470.86 1487.50 1488.14 1488.69
 1493.66 1499.85 1501.89 1503.85 1504.92 1506.14
 1508.05 1511.32 1512.99 1516.15 1517.74 1520.69
 1521.90 1524.13 1535.10 1535.86 1536.47 1539.61
 1584.89 1591.81 1601.57 1607.10 1619.98 1622.80
 1653.76 2068.14 2924.32 2968.41 3040.79 3042.96
 3043.91 3044.98 3045.92 3046.82 3050.69 3052.51
 3053.21 3110.93 3112.39 3114.21 3116.14 3117.00
 3120.55 3120.76 3122.39 3122.79 3130.54 3130.72
 3131.93 3141.65 3143.36 3143.52 3147.10 3147.70
 3150.41 3165.59 3168.00 3172.27 3174.35 3174.91
 3183.85 3189.53 3193.92 3198.83 3200.98 3208.16
 3305.41 3306.15 3308.55 3326.14 3327.68 3330.19

¹a (R=Bu)

 5.89 27.58 32.09 35.87 39.82 41.63
 46.41 51.62 58.69 65.83 69.31 76.64
 79.17 81.99 89.08 102.80 127.92 131.87
 144.99 150.98 164.41 179.75 184.24 194.51
 201.93 205.62 209.24 219.62 241.25 244.49
 248.20 256.20 257.85 261.50 265.52 282.60
 286.83 298.02 299.72 302.40 311.92 320.16
 324.56 343.95 344.81 348.10 350.27 352.92
 354.15 360.09 366.35 369.04 387.72 391.41
 397.13 406.81 411.64 414.53 416.08 427.65
 459.31 464.27 466.27 477.26 490.58 498.52
 501.77 516.09 528.31 552.15 591.22 598.87
 602.49 609.61 626.63 632.06 637.08 639.06
 645.86 661.34 687.63 693.97 706.12 707.63
 715.73 720.34 728.12 731.43 735.65 754.26
 771.20 796.89 804.63 821.81 824.70 828.26
 828.87 830.41 831.36 834.07 838.33 884.39
 890.89 893.69 936.11 937.03 938.02 941.72
 942.54 943.89 950.85 952.82 962.02 977.36
 980.06 981.44 984.10 994.05 998.12 1004.96
 1007.58 1010.13 1012.50 1017.96 1035.55 1039.32
 1043.82 1044.38 1058.78 1059.13 1061.67 1066.14
 1067.36 1068.17 1070.39 1071.44 1109.17 1109.71
 1118.86 1137.98 1139.33 1153.25 1176.20 1177.78
 1180.17 1181.84 1188.56 1193.71 1201.99 1207.63
 1224.08 1225.77 1227.35 1240.82 1250.55 1252.41
 1256.63 1257.90 1260.08 1261.23 1262.70 1283.92
 1295.86 1300.76 1304.46 1307.13 1312.06 1316.56
 1317.53 1341.48 1361.80 1368.54 1371.51 1373.81
 1391.62 1409.41 1412.33 1413.50 1413.93 1415.46
 1416.28 1426.77 1427.98 1441.57 1442.34 1442.98
 1443.51 1445.81 1472.17 1477.69 1486.42 1487.59
 1487.70 1494.81 1504.31 1504.75 1505.94 1508.29
 1509.97 1510.63 1512.46 1513.66 1515.88 1518.42
 1522.57 1524.07 1526.07 1537.02 1538.00 1540.06
 1543.99 1593.35 1610.59 1612.92 1615.89 1617.98
 1624.38 1655.37 2929.94 2977.22 3040.96 3041.86
 3043.24 3043.82 3044.61 3045.72 3051.11 3051.45

3052.27 3110.42 3110.84 3113.24 3113.60 3113.88
 3118.79 3120.68 3122.00 3122.61 3129.04 3130.14
 3130.71 3145.43 3147.70 3148.61 3151.46 3152.81
 3158.14 3162.87 3167.74 3169.78 3175.93 3176.29
 3186.68 3190.07 3197.11 3200.87 3202.56 3208.08
 3306.72 3309.26 3309.87 3333.26 3333.61 3333.86

³a-TS (R=Bu)

 -374.30 12.12 28.77 38.52 41.35 44.77
 48.21 52.58 61.73 62.47 67.89 72.60
 79.46 86.21 90.06 91.20 101.23 129.51
 131.27 144.24 150.59 158.08 176.86 182.05
 195.87 202.26 208.77 225.72 236.63 240.68
 252.99 254.75 257.23 260.32 265.57 272.21
 287.54 295.13 296.30 299.05 301.73 315.27
 328.74 338.74 341.14 346.21 346.53 350.52
 353.45 359.61 364.15 367.95 380.35 386.45
 390.35 404.91 412.29 412.87 417.10 423.77
 429.28 460.56 465.26 466.40 487.16 498.54
 502.26 510.91 515.07 523.40 560.97 596.18
 600.40 603.49 629.91 632.21 638.72 641.52
 648.13 659.46 693.82 695.01 707.04 711.27
 713.88 718.34 724.74 728.17 737.29 753.84
 769.94 796.53 804.61 820.82 828.48 828.95
 830.55 831.64 832.50 839.57 840.33 885.91
 890.96 892.83 936.18 936.46 937.80 940.77
 941.31 943.69 954.21 959.63 976.01 978.34
 981.75 983.32 993.77 1000.21 1004.86 1006.43
 1007.99 1008.36 1011.18 1016.53 1034.64 1038.60
 1041.04 1049.67 1058.10 1058.55 1059.88 1065.72
 1066.96 1068.51 1068.98 1075.34 1109.43 1117.11
 1138.15 1140.16 1148.00 1169.05 1175.09 1176.53
 1180.91 1182.62 1186.68 1188.51 1199.31 1204.51
 1223.79 1225.27 1227.34 1239.40 1249.27 1250.48
 1253.85 1256.46 1260.37 1261.16 1262.96 1284.83
 1293.66 1294.22 1302.62 1306.03 1307.54 1315.75
 1317.26 1342.94 1365.34 1366.78 1367.34 1371.17
 1383.25 1410.04 1411.65 1413.71 1414.49 1415.98
 1418.59 1426.53 1428.31 1434.74 1441.92 1442.60
 1443.27 1447.42 1472.25 1486.15 1487.69 1488.27
 1490.67 1497.97 1499.16 1504.44 1506.76 1507.72
 1508.91 1510.03 1512.06 1512.99 1515.25 1520.74
 1523.50 1524.34 1528.87 1535.56 1537.01 1539.45
 1542.69 1605.56 1608.38 1611.56 1613.82 1624.28
 1633.38 1655.65 2959.12 3001.21 3041.23 3043.31
 3044.95 3045.49 3045.97 3046.60 3051.94 3052.37
 3052.94 3110.07 3111.18 3114.30 3114.69 3116.99
 3119.82 3120.81 3122.93 3123.14 3128.38 3129.66
 3131.09 3145.54 3150.20 3152.78 3156.62 3159.43
 3165.90 3167.02 3167.78 3173.72 3175.65 3183.63
 3189.72 3196.44 3198.21 3202.34 3205.13 3207.92
 3308.35 3310.08 3310.66 3331.31 3331.41 3333.17

¹a-TS (R=Bu)

 -402.79 22.40 30.46 38.27 39.71 47.43
 48.72 57.68 59.24 63.85 70.18 78.58
 82.02 90.01 98.83 104.09 109.68 130.22
 141.94 153.13 156.49 171.22 178.57 181.92
 199.63 205.35 222.18 229.55 232.98 242.58
 253.94 255.17 259.38 267.13 269.50 279.88
 290.58 297.21 300.90 308.25 310.68 322.63
 337.71 348.33 349.89 350.99 351.80 356.35
 358.05 367.68 370.24 382.53 387.48 399.02
 401.71 411.68 414.66 417.43 417.93 428.83
 429.52 463.53 466.96 469.55 483.73 498.16
 502.74 509.15 516.19 524.97 564.19 597.06
 602.17 605.29 629.52 632.28 640.84 643.41
 651.35 660.77 696.02 698.27 708.81 713.35

720.34	729.79	730.77	731.67	738.10	756.99	3045.63	3046.85	3047.02	3047.46	3053.24	3053.74
774.94	795.70	807.08	823.91	827.41	829.70	3054.26	3080.06	3113.22	3115.39	3115.91	3117.54
832.41	833.60	834.04	841.14	843.46	885.32	3118.51	3120.70	3121.50	3122.73	3122.86	3130.58
890.26	898.00	936.55	937.37	938.55	939.12	3131.22	3131.82	3139.44	3143.22	3146.74	3147.00
939.61	942.44	953.12	963.23	976.01	979.35	3151.62	3153.06	3161.17	3168.33	3170.99	3175.19
979.98	985.62	995.02	999.98	1002.88	1004.86	3181.01	3189.87	3193.94	3194.34	3200.98	3201.28
1006.66	1010.59	1013.88	1016.45	1036.70	1041.51	3305.20	3305.58	3308.58	3325.21	3326.27	3328.65
1044.73	1049.92	1056.50	1057.07	1057.24	1060.55	*****	*****	*****	*****	*****	*****
1065.47	1067.93	1068.48	1071.67	1108.08	1111.13	³2 (R="Bu)					
1137.11	1139.02	1144.42	1148.71	1178.88	1181.29	*****					
1181.71	1185.32	1185.86	1187.48	1198.62	1203.61	16.81	29.04	37.33	38.16	40.00	47.38
1226.49	1228.26	1230.36	1237.70	1239.18	1243.59	48.45	50.21	51.09	59.91	60.92	71.27
1246.24	1255.77	1260.78	1261.73	1262.74	1288.29	74.68	83.19	85.07	116.25	118.29	145.04
1288.84	1293.58	1303.82	1304.92	1308.18	1315.44	149.19	168.19	174.94	209.00	209.55	213.26
1320.34	1342.66	1359.91	1361.95	1364.39	1370.20	216.26	218.57	223.76	231.47	233.72	234.21
1377.98	1409.26	1410.42	1412.77	1414.11	1414.85	235.76	240.50	241.92	244.49	247.54	249.66
1416.37	1431.16	1433.19	1433.48	1441.60	1442.71	254.26	260.93	279.47	281.08	303.58	326.49
1445.19	1449.50	1470.91	1486.15	1487.08	1488.33	336.93	349.49	353.11	356.69	360.68	369.29
1493.44	1497.45	1504.30	1505.38	1506.53	1507.35	374.50	376.40	382.87	393.09	394.59	394.98
1509.80	1511.46	1512.13	1513.94	1515.58	1521.21	408.08	409.66	432.48	448.73	449.08	459.64
1523.83	1527.00	1528.05	1535.70	1536.52	1540.15	473.95	496.96	522.47	534.39	540.37	545.85
1545.62	1605.72	1605.83	1612.38	1622.57	1623.20	546.81	562.18	568.21	613.06	620.39	625.39
1630.78	1654.17	2970.32	3012.22	3040.69	3041.67	644.90	648.37	675.92	688.18	697.54	719.00
3044.41	3044.68	3044.98	3046.64	3051.56	3051.81	735.78	764.78	784.82	787.99	789.54	804.94
3053.03	3107.68	3109.29	3110.92	3112.28	3117.45	850.58	851.73	857.36	860.00	891.48	904.04
3120.21	3123.06	3123.65	3123.78	3126.57	3129.10	909.98	913.72	929.67	936.29	937.58	938.34
3131.78	3144.52	3147.39	3149.40	3157.15	3158.34	965.90	971.41	975.75	982.99	983.45	989.30
3167.97	3168.85	3171.57	3175.10	3175.65	3186.55	1000.77	1005.35	1013.84	1023.82	1024.61	1024.87
3190.15	3195.76	3201.52	3202.04	3208.04	3215.43	1026.07	1026.48	1026.54	1028.39	1033.70	1035.13
3307.99	3308.14	3308.40	3332.04	3333.80	3336.89	1035.89	1043.10	1057.56	1067.91	1073.60	1093.25
*****	*****	*****	*****	*****	*****	1136.44	1140.82	1171.41	1187.68	1191.33	1193.12
⁵2 (R="Bu)						1195.05	1200.25	1230.57	1231.92	1236.02	1244.03
*****						1255.94	1258.19	1268.08	1276.89	1277.12	1278.15
1.56	28.21	30.88	34.70	40.23	41.61	1280.37	1302.07	1304.55	1309.09	1309.39	1310.37
46.10	46.22	56.59	62.04	67.88	68.66	1331.84	1341.43	1351.41	1371.26	1388.77	1396.82
76.96	78.74	81.38	96.71	113.04	123.07	1397.05	1419.09	1419.68	1464.20	1469.83	1478.97
130.70	132.44	144.73	164.31	172.71	174.21	1483.26	1498.75	1507.50	1511.78	1568.77	1577.49
181.66	199.75	205.19	206.64	216.08	218.00	1584.63	1593.88	1607.51	1608.79	1610.33	1613.17
242.26	245.05	247.02	253.88	256.50	257.55	1617.38	1620.93	1622.00	1626.47	1627.14	1627.56
282.75	284.98	291.01	293.69	299.10	304.35	1629.30	1635.88	1636.63	1638.47	1647.80	1648.42
328.93	333.39	336.06	338.32	340.70	345.96	1649.08	1649.92	1654.02	1654.15	1655.37	1655.38
351.05	356.34	359.45	365.51	372.04	378.00	1655.95	1657.45	1657.47	1657.76	1657.88	1660.19
378.81	399.45	406.83	411.09	420.76	430.43	1660.27	1662.03	1664.98	1665.94	1666.28	1682.14
445.41	458.61	462.82	463.44	499.63	503.74	1683.09	1705.78	1705.89	1711.12	1731.53	1732.93
511.26	520.32	557.83	594.26	598.16	600.51	1733.72	1734.46	1747.57	1747.63	1774.00	1775.03
601.19	631.29	631.56	640.65	644.13	650.24	1775.54	1778.41	1789.36	1838.65	1843.57	1844.18
658.29	687.45	702.81	707.50	714.78	719.00	1857.08	1988.53	3021.00	3021.01	3021.14	3022.08
725.33	726.81	737.07	751.74	764.09	778.83	3022.27	3022.56	3022.62	3022.86	3024.05	3061.14
804.41	822.46	826.42	827.66	830.88	831.27	3105.03	3130.51	3131.81	3132.41	3133.18	3133.94
838.78	847.54	860.56	883.27	884.70	886.39	3135.48	3135.66	3135.87	3136.02	3136.13	3137.03
922.48	929.89	933.38	934.61	935.08	941.27	3137.27	3137.30	3138.52	3138.89	3139.39	3140.93
942.70	943.35	954.40	966.93	975.54	977.90	3144.11	3144.83	3145.23	3146.66	3147.69	3147.72
979.25	990.26	999.04	1000.88	1003.45	1004.61	3148.38	3148.99	3149.61	3150.38	3150.56	3152.30
1007.52	1008.00	1012.60	1013.49	1031.07	1035.34	3197.71	3199.49	3199.98	3203.71	3204.38	3205.20
1037.08	1054.24	1057.81	1058.19	1058.71	1059.49	*****	*****	*****	*****	*****	*****
1062.92	1063.63	1064.50	1067.37	1103.29	1108.58	¹2 (R="Bu)					
1109.36	1137.59	1138.63	1143.44	1146.03	1169.03	*****					
1169.94	1177.23	1184.35	1187.74	1189.41	1201.20	18.93	31.74	39.01	42.20	46.08	46.47
1220.78	1221.50	1222.82	1226.86	1234.72	1251.05	51.78	62.81	71.83	76.35	80.75	83.02
1253.17	1255.96	1259.81	1260.94	1261.70	1286.50	89.06	104.47	110.36	113.48	127.29	135.52
1289.64	1294.63	1305.34	1306.60	1307.99	1315.76	141.56	153.51	173.41	180.02	181.46	199.75
1319.58	1337.07	1363.09	1365.98	1369.45	1371.02	205.51	208.31	221.98	231.32	248.90	250.81
1382.60	1411.81	1413.33	1414.98	1415.47	1417.44	256.06	261.13	264.48	272.99	281.84	286.77
1417.78	1420.33	1424.82	1428.47	1440.37	1443.65	293.72	300.27	301.11	312.44	322.44	330.35
1445.49	1447.24	1470.53	1486.98	1487.95	1490.00	340.58	344.45	346.81	348.05	353.41	358.62
1494.46	1497.96	1498.49	1501.72	1503.06	1504.96	362.81	371.06	375.52	383.43	390.46	396.70
1507.60	1510.56	1510.61	1513.97	1519.16	1519.60	403.13	407.16	416.27	422.97	423.62	430.52
1521.97	1530.78	1534.63	1535.84	1536.28	1537.72	437.39	462.74	469.94	472.45	497.00	503.64
1539.33	1600.70	1606.63	1612.33	1621.96	1638.42	516.00	524.34	555.65	592.32	595.00	601.36
1653.41	1660.66	3016.17	3027.03	3043.24	3045.43	603.58	627.60	630.56	638.80	642.89	650.06

659.23 694.21 705.05 705.90 713.81 715.75
729.73 736.32 738.53 755.79 758.09 779.04
811.02 823.01 824.94 827.06 828.50 831.22
832.30 834.76 842.56 859.73 885.22 887.85
922.32 934.88 936.00 936.82 937.64 938.95
941.79 942.40 952.91 970.41 973.06 975.85
982.92 991.55 996.16 999.46 999.56 1000.62
1003.36 1004.67 1007.02 1014.75 1036.00 1042.23
1046.99 1052.06 1056.08 1057.38 1058.61 1059.74
1065.17 1066.67 1071.31 1074.77 1106.17 1108.45
1116.54 1134.87 1137.52 1141.22 1148.50 1179.70
1180.97 1185.30 1185.62 1187.82 1195.17 1204.45
1218.64 1226.17 1226.96 1229.84 1230.93 1237.43
1241.22 1246.55 1260.86 1262.39 1263.26 1277.14
1280.96 1294.51 1300.39 1306.84 1307.73 1314.55
1324.47 1334.27 1357.69 1364.49 1366.02 1370.69
1386.93 1409.41 1411.02 1412.43 1412.94 1414.14
1415.14 1417.89 1431.55 1432.01 1441.49 1442.92
1445.27 1450.54 1470.55 1485.67 1487.14 1489.09
1490.26 1494.48 1499.73 1501.99 1503.76 1506.49
1508.22 1509.35 1510.99 1516.84 1519.38 1521.29
1526.11 1530.22 1532.61 1536.06 1537.08 1539.92
1546.66 1609.54 1612.47 1622.03 1625.15 1637.07
1653.39 1659.33 3029.67 3039.55 3042.39 3046.44
3047.07 3047.79 3048.60 3053.25 3054.29 3055.04
3072.67 3096.90 3106.26 3110.97 3111.31 3117.51
3120.11 3123.13 3124.37 3124.88 3125.28 3128.60
3129.15 3131.50 3138.69 3145.60 3153.16 3155.26
3157.29 3163.54 3167.39 3172.65 3174.72 3183.11
3189.96 3190.71 3196.55 3197.45 3202.96 3206.31
3302.45 3309.03 3311.94 3328.27 3331.71 3338.46

⁵1 (R=H)

42.08 59.11 64.60 68.95 89.31 109.05
114.26 130.89 166.50 167.31 186.46 191.53
208.95 237.26 241.92 259.67 278.42 297.32
323.38 324.76 348.85 353.88 373.15 425.45
506.36 604.93 614.72 623.55 633.90 652.90
654.08 659.97 674.28 697.66 703.54 711.23
728.35 731.00 731.68 734.47 751.27 796.75
821.06 839.49 842.12 847.42 867.38 884.37
892.87 943.26 944.12 946.31 953.08 995.73
1003.58 1003.62 1008.40 1009.49 1016.11 1063.61
1105.34 1106.27 1108.52 1110.37 1128.90 1130.38
1134.97 1187.50 1196.79 1203.28 1209.29 1222.25
1229.84 1246.22 1251.34 1266.35 1293.88 1296.54
1319.45 1322.58 1368.18 1416.84 1423.63 1435.67
1460.50 1462.77 1467.75 1471.71 1537.27 1598.56
1601.98 1608.69 1623.58 1655.07 3173.78 3180.47
3193.10 3197.55 3205.73 3294.13 3294.25 3295.58
3319.65 3320.30 3321.69 3666.02 3667.61 3677.50

³1 (R=H)

34.70 41.97 61.37 64.96 69.41 106.13
138.04 150.75 169.61 173.36 192.68 195.73
210.57 236.29 255.37 307.00 316.57 319.97
333.00 348.80 360.79 371.45 391.37 424.59
505.23 604.37 609.93 615.20 634.11 651.48
654.45 657.82 662.43 692.50 703.77 709.44
723.98 727.31 731.74 734.51 753.71 795.90
819.75 832.24 840.17 846.97 883.12 895.29
943.96 944.87 947.63 952.49 994.18 1003.31
1005.82 1011.28 1016.48 1018.56 1063.97 1090.10
1100.93 1103.58 1106.87 1108.09 1128.62 1129.68
1137.89 1187.39 1198.69 1210.28 1216.37 1223.10
1235.37 1244.19 1250.70 1265.38 1288.76 1304.20
1318.49 1329.91 1367.67 1418.63 1423.62 1438.84
1459.82 1470.22 1472.12 1479.46 1537.18 1600.67

1603.36 1607.24 1623.20 1654.58 3173.65 3181.25
3194.37 3199.96 3206.20 3293.34 3296.38 3296.80
3319.05 3319.77 3320.72 3676.66 3682.56 3683.18

¹1 (R=H)

41.55 64.06 67.48 70.26 112.01 156.39
162.45 164.21 179.67 184.96 201.20 201.25
224.23 243.02 257.76 314.35 323.12 324.91
360.38 370.69 386.42 422.49 426.99 428.35
506.39 576.19 586.04 592.66 631.97 634.24
635.15 638.98 655.59 682.43 697.51 701.82
715.08 721.32 727.81 736.02 754.20 789.77
814.32 831.57 834.51 840.29 885.64 896.80
943.99 944.33 945.97 954.87 996.67 1005.00
1006.20 1009.58 1015.45 1016.85 1064.71 1095.04
1098.87 1102.74 1108.25 1128.34 1131.34 1141.31
1188.80 1196.92 1202.83 1203.29 1210.55 1225.35
1232.42 1246.71 1251.24 1269.75 1280.99 1290.19
1317.42 1318.15 1369.23 1415.30 1415.55 1428.41
1471.91 1484.22 1486.68 1497.95 1538.40 1606.86
1608.19 1611.55 1624.63 1655.96 3167.46 3175.61
3188.75 3195.36 3200.72 3291.69 3292.41 3292.48
3313.59 3317.87 3318.04 3690.17 3690.33 3690.89

⁵1a (R=H)

18.20 24.06 30.61 40.25 47.69 59.81
63.88 66.48 80.74 96.31 111.05 136.54
157.97 162.53 165.48 178.05 188.84 193.62
211.83 235.94 241.28 254.85 260.55 294.40
299.43 317.05 328.71 343.20 351.70 361.11
376.41 412.87 426.28 474.19 490.60 507.47
544.06 548.57 602.94 611.72 615.98 626.24
635.38 649.29 651.83 663.60 678.90 683.86
699.37 704.52 709.08 709.80 726.30 729.34
735.49 741.62 753.01 767.07 789.43 795.11
823.02 832.38 839.57 842.95 851.20 886.12
888.33 893.94 928.88 942.09 943.15 946.12
953.66 964.48 984.26 992.15 996.96 1002.63
1004.82 1008.77 1014.73 1016.97 1038.58 1053.35
1064.54 1072.74 1104.38 1107.26 1108.48 1109.69
1112.00 1125.99 1126.72 1136.36 1178.48 1188.70
1191.70 1197.29 1201.01 1205.56 1213.81 1223.76
1232.03 1241.00 1250.86 1252.44 1265.58 1286.30
1295.91 1307.70 1318.91 1323.38 1336.84 1360.51
1369.84 1416.95 1417.59 1432.44 1434.65 1454.16
1458.27 1463.50 1472.91 1482.03 1491.02 1516.31
1537.87 1586.62 1601.92 1605.99 1612.64 1614.85
1624.90 1655.63 2956.30 2979.30 3156.88 3168.18
3171.83 3175.97 3176.77 3188.75 3188.81 3194.59
3201.02 3202.31 3209.60 3288.42 3290.59 3291.73
3316.35 3317.16 3319.29 3603.46 3675.54 3680.94

³1a (R=H)

15.85 29.95 34.12 41.02 43.68 61.15
65.63 67.92 87.06 110.60 141.19 157.38
173.06 176.17 191.90 199.98 209.93 215.15
234.35 250.26 255.23 271.50 318.51 324.62
338.18 343.35 358.30 371.20 391.35 393.87
413.73 424.14 427.49 484.84 504.09 522.18
570.11 601.84 610.41 620.13 625.09 635.31
637.90 648.90 653.92 658.59 686.17 689.73
700.00 705.16 708.99 709.42 725.02 727.09
735.83 743.92 753.10 772.64 794.15 799.94
820.84 830.22 838.93 839.52 847.04 884.48
891.55 898.35 943.15 944.40 947.80 952.57
965.49 973.14 985.00 996.01 997.53 1005.10
1009.86 1014.03 1017.49 1027.23 1043.29 1064.07

1065.03 1103.25 1107.50 1108.10 1108.54 1115.34
1125.15 1126.00 1130.35 1137.63 1180.46 1188.42
1195.54 1202.98 1208.57 1215.34 1222.31 1224.50
1234.04 1241.76 1244.26 1256.36 1268.17 1294.59
1307.93 1320.24 1322.62 1335.25 1341.61 1362.49
1369.10 1423.39 1425.36 1434.76 1444.40 1455.19
1464.36 1472.85 1476.56 1483.19 1493.95 1519.67
1538.34 1591.74 1599.13 1601.67 1607.54 1617.11
1624.98 1656.04 2966.94 2992.69 3166.36 3168.20
3172.12 3175.90 3177.64 3188.81 3189.25 3194.74
3201.12 3201.98 3210.85 3289.52 3291.08 3292.60
3313.42 3314.06 3315.76 3609.65 3676.79 3686.59

¹a (R=H)

15.93 29.37 37.28 38.76 43.07 61.77
66.56 68.86 84.47 110.15 141.07 159.19
173.50 181.18 200.23 202.21 210.32 217.61
234.49 247.37 254.51 268.16 319.54 324.82
342.99 349.87 361.76 371.65 388.85 389.29
414.01 423.19 425.70 484.11 505.20 548.06
557.85 604.52 614.26 620.41 626.43 635.80
648.67 651.06 656.01 660.07 675.49 689.06
697.43 706.87 710.55 717.38 724.79 727.94
736.69 740.82 758.26 768.78 799.37 803.01
822.53 831.02 835.14 840.60 848.38 884.71
886.54 898.80 943.32 944.38 947.85 952.87
961.71 962.58 984.50 994.71 995.27 1005.06
1009.43 1013.32 1017.26 1026.97 1042.90 1065.15
1067.57 1103.40 1107.53 1108.18 1108.50 1118.64
1128.31 1129.81 1130.79 1138.42 1179.09 1188.43
1192.82 1201.76 1206.09 1215.37 1222.49 1225.59
1234.93 1242.20 1242.71 1258.19 1266.73 1294.60
1306.50 1316.48 1321.17 1333.39 1338.66 1360.84
1369.04 1423.40 1424.64 1441.28 1443.80 1455.16
1462.24 1472.54 1473.52 1482.67 1493.94 1517.49
1538.35 1588.56 1598.81 1602.61 1610.15 1616.22
1624.61 1655.91 2960.57 3011.99 3161.70 3168.06
3171.35 3175.88 3175.97 3188.27 3188.40 3194.49
3197.29 3200.78 3205.15 3289.12 3291.32 3292.34
3312.92 3313.50 3315.88 3645.01 3675.85 3683.63

⁵1-TS (R=H)

-385.03 10.07 24.40 31.34 41.11 44.43
56.91 64.05 65.59 78.53 90.02 108.83
120.95 131.59 163.43 163.63 183.46 185.92
193.90 216.33 228.93 241.37 247.77 262.33
268.15 296.74 310.60 319.04 320.35 347.06
350.11 363.31 417.24 427.84 447.73 491.75
508.04 558.76 612.34 619.93 622.81 629.32
632.68 650.37 656.61 671.08 673.31 678.11
694.68 699.98 711.59 715.24 718.78 729.93
732.04 735.44 738.35 751.76 791.74 793.49
797.58 821.83 840.79 843.87 850.00 850.82
886.14 887.62 908.22 942.56 943.36 944.88
946.38 947.04 954.71 968.52 986.30 998.06
1002.51 1003.78 1006.41 1006.87 1012.72 1013.92
1039.64 1055.99 1062.77 1105.51 1108.59 1109.22
1114.12 1114.23 1129.42 1130.35 1136.04 1183.18
1188.67 1194.60 1202.40 1206.37 1209.87 1222.47
1229.79 1235.64 1249.28 1258.25 1268.20 1288.71
1294.68 1303.38 1319.01 1319.81 1345.33 1365.26
1369.88 1419.92 1420.62 1434.35 1448.89 1457.15
1461.51 1472.19 1474.70 1488.27 1531.07 1536.86
1592.07 1600.23 1603.47 1609.37 1621.03 1624.72
1647.21 1655.56 3155.20 3168.69 3169.52 3176.27
3176.92 3185.45 3187.57 3189.34 3194.72 3197.51
3201.68 3211.61 3270.73 3289.71 3290.45 3290.50
3317.02 3317.47 3318.12 3606.77 3673.11 3673.97

³1-TS (R=H)

-395.22 15.97 25.01 33.48 40.92 43.17
61.71 66.63 67.49 85.78 109.00 139.29
154.81 173.18 175.26 181.89 193.25 199.09
208.77 230.15 244.23 253.93 267.71 308.80
325.48 328.89 336.39 356.22 361.98 374.92
384.74 417.95 420.82 424.54 463.59 505.70
508.81 557.06 605.91 612.51 623.88 629.68
635.86 650.47 654.50 660.16 692.26 695.09
707.39 710.19 717.18 725.29 727.46 728.77
735.97 750.29 754.07 786.51 789.92 798.32
821.63 834.03 835.49 842.27 850.65 850.81
885.45 898.18 899.53 937.35 943.39 944.95
947.39 953.65 964.62 985.93 995.44 1003.54
1005.52 1008.31 1012.70 1017.20 1027.28 1047.85
1062.89 1065.51 1077.98 1103.97 1107.96 1109.11
1112.77 1114.35 1129.67 1131.55 1137.47 1182.54
1189.25 1201.95 1205.28 1213.23 1220.83 1224.55
1233.32 1239.48 1243.60 1255.28 1275.31 1287.93
1293.60 1306.78 1320.32 1332.25 1340.53 1365.42
1369.32 1421.50 1425.41 1441.46 1443.69 1460.52
1470.61 1473.32 1484.90 1486.49 1528.91 1538.50
1564.27 1601.12 1603.66 1609.17 1612.73 1625.19
1643.49 1655.96 3149.97 3157.81 3167.45 3169.35
3173.52 3177.22 3184.66 3189.50 3195.61 3198.15
3201.92 3204.85 3236.52 3290.73 3293.78 3295.19
3315.53 3315.72 3318.09 3573.39 3676.26 3686.58

¹1-TS (CSS) (R=H)

-494.94 14.43 28.77 33.16 41.90 47.42
54.65 67.46 69.60 75.00 113.13 148.34
160.61 176.08 183.03 190.68 197.28 208.21
228.80 246.48 250.98 256.23 271.26 314.43
328.13 336.02 346.07 362.45 379.13 389.38
414.74 417.27 424.78 449.08 466.97 508.06
513.67 561.56 567.92 586.65 606.62 629.74
631.63 635.70 637.30 655.55 662.51 683.37
695.94 697.23 698.95 714.51 722.86 727.95
734.47 737.59 758.12 771.35 794.14 798.91
810.94 817.36 825.76 833.13 839.30 846.08
884.06 897.60 910.11 942.81 943.18 946.08
952.63 958.07 966.92 991.26 995.01 1004.38
1006.85 1007.54 1012.38 1017.09 1023.51 1049.95
1065.20 1065.98 1098.79 1100.74 1102.55 1107.06
1113.52 1122.49 1128.34 1129.64 1140.55 1185.71
1188.39 1200.28 1207.37 1207.94 1216.03 1223.67
1233.09 1236.66 1238.77 1244.77 1262.10 1277.27
1293.53 1295.32 1318.46 1323.72 1346.83 1368.10
1368.49 1414.07 1418.49 1433.09 1450.35 1470.16
1474.60 1477.32 1487.16 1490.15 1530.82 1538.17
1575.91 1606.28 1607.08 1610.70 1619.55 1624.96
1647.42 1655.79 3153.87 3167.56 3169.36 3172.93
3175.97 3180.03 3188.47 3189.08 3196.01 3201.41
3201.95 3216.69 3232.98 3290.95 3291.21 3292.55
3314.42 3316.05 3316.63 3643.45 3687.82 3692.24

¹1-TS (OSS) (R=H)

-750.29 13.13 26.72 29.25 41.41 43.78
56.05 66.52 69.63 72.10 111.73 135.48
157.39 170.77 177.21 189.02 193.41 201.03
206.50 225.71 243.59 253.56 259.83 309.95
314.51 327.49 337.59 358.99 372.95 385.43
389.97 417.82 423.86 429.71 452.58 504.02
505.96 558.91 572.22 588.54 601.75 629.62
631.70 635.64 638.01 645.39 655.03 683.16
693.67 695.04 699.48 708.95 713.98 722.62

728.12 730.68 735.96 756.01 786.48 791.49
800.16 816.68 828.00 833.43 839.70 845.83
883.92 897.28 909.39 942.86 943.54 946.24
947.67 952.82 967.85 990.28 994.99 1004.27
1005.06 1006.05 1011.10 1016.71 1021.06 1047.74
1063.56 1064.99 1081.92 1098.66 1101.01 1102.58
1107.17 1116.43 1128.06 1129.62 1140.56 1184.33
1188.57 1199.58 1205.06 1206.16 1214.58 1224.01
1231.16 1234.74 1236.32 1246.24 1262.38 1276.42
1285.65 1294.49 1318.28 1322.25 1343.89 1366.02
1368.65 1413.58 1417.22 1431.68 1443.75 1470.76
1475.24 1478.21 1486.45 1488.61 1528.63 1538.28
1561.97 1606.35 1606.78 1610.35 1616.69 1625.14
1643.22 1655.85 3157.32 3161.74 3168.18 3168.62
3176.94 3178.82 3186.54 3189.82 3196.51 3202.34
3202.49 3215.66 3239.49 3292.04 3292.38 3292.75
3313.86 3316.85 3318.04 3665.80 3688.46 3692.58

³1a-TS (R=H)

-404.29 13.42 23.51 42.48 43.27 47.96
61.98 64.04 68.91 80.05 110.29 143.67
152.28 172.66 173.34 193.68 195.07 207.13
211.91 235.04 254.71 257.30 280.96 309.29
322.48 331.31 340.72 352.99 368.15 369.52
374.28 415.70 425.93 426.90 505.18 507.42
528.36 558.32 586.95 595.62 614.22 629.61
632.52 638.93 645.32 652.68 668.69 688.25
693.07 700.90 702.10 707.00 717.98 723.16
732.04 735.51 752.81 767.45 792.76 794.64
817.58 829.23 835.72 842.01 842.26 884.56
890.11 892.09 942.46 943.20 945.80 953.32
965.05 982.98 992.12 997.26 1003.74 1005.07
1007.30 1008.92 1014.95 1017.46 1048.16 1062.58
1072.38 1100.18 1103.96 1105.13 1107.81 1119.28
1126.34 1128.70 1136.96 1160.91 1181.34 1188.52
1193.22 1199.20 1204.86 1208.55 1215.65 1223.45
1235.05 1237.66 1244.82 1256.50 1262.48 1283.97
1295.14 1298.36 1318.72 1322.60 1339.40 1363.57
1369.47 1415.37 1417.59 1432.09 1434.07 1466.53
1470.96 1472.89 1479.96 1491.51 1501.77 1527.93
1537.48 1599.61 1603.52 1605.30 1608.54 1624.77
1631.49 1655.68 2981.41 3015.83 3167.87 3168.42
3176.16 3176.24 3185.00 3189.39 3195.77 3200.65
3201.93 3202.39 3208.87 3290.93 3291.69 3291.81
3314.35 3317.72 3318.52 3629.26 3684.11 3689.07

¹1a-TS (R=H)

-401.47 8.23 31.58 35.79 44.48 51.90
62.54 66.00 68.34 83.16 111.49 149.90
166.64 172.87 180.84 197.07 198.38 211.79
223.07 242.24 251.29 258.79 283.66 323.43
340.94 349.62 359.70 368.08 374.72 399.58
415.82 418.23 424.61 426.99 504.63 507.01
530.84 560.79 595.22 606.30 615.14 629.45
634.42 644.62 651.70 657.53 660.07 692.80
695.84 704.95 708.52 710.84 722.39 726.25
736.48 737.11 755.45 770.91 789.71 799.72
820.60 832.08 836.75 845.14 845.31 884.15
897.65 898.13 942.56 943.43 946.55 952.28
968.41 987.54 990.20 995.18 1004.85 1009.12
1011.90 1014.47 1017.87 1026.24 1049.29 1062.49
1065.59 1102.25 1105.62 1106.99 1107.93 1118.67
1126.89 1127.17 1134.47 1142.20 1178.26 1185.49
1188.25 1201.11 1203.61 1215.54 1221.16 1223.45
1228.54 1236.45 1241.86 1252.54 1263.26 1287.56
1289.97 1302.90 1320.58 1331.08 1338.45 1362.80
1368.66 1421.50 1422.51 1429.48 1443.19 1455.70
1464.83 1472.76 1473.51 1491.48 1504.37 1525.84

1538.24 1599.56 1601.00 1602.41 1606.47 1625.00
1629.04 1656.50 2973.38 3008.42 3167.83 3170.63
3175.50 3178.12 3187.48 3188.34 3194.21 3200.73
3200.99 3206.90 3210.08 3288.56 3290.37 3290.78
3310.80 3313.15 3315.63 3642.45 3676.70 3687.16

⁵2 (R=H)

15.82 21.16 23.27 39.76 44.84 60.52
63.96 65.30 74.75 90.44 105.41 133.92
143.84 164.68 165.33 175.08 188.44 195.84
204.45 214.52 242.31 248.33 263.22 294.34
313.48 316.36 331.56 339.35 345.98 360.64
388.02 420.90 427.99 434.32 509.49 554.93
590.97 594.92 606.52 617.17 632.73 633.03
646.15 649.74 660.19 675.73 694.93 708.15
711.43 716.83 724.04 728.61 735.06 743.76
749.63 763.58 776.15 794.36 820.10 836.49
841.80 851.54 866.30 872.35 886.19 887.54
924.70 940.91 941.99 944.62 951.39 954.10
974.33 992.92 997.08 1000.65 1002.75 1005.77
1009.65 1011.88 1013.15 1016.25 1048.59 1055.27
1062.32 1099.73 1104.05 1104.92 1106.93 1107.89
1108.84 1122.52 1127.79 1130.44 1136.42 1183.02
1188.44 1191.97 1197.47 1202.27 1207.33 1222.43
1226.57 1228.60 1239.06 1246.62 1260.80 1276.24
1291.58 1297.64 1317.15 1318.88 1338.38 1360.96
1370.04 1412.63 1416.00 1417.10 1429.34 1458.98
1463.26 1472.18 1474.30 1493.38 1524.20 1534.72
1536.94 1603.97 1606.20 1610.09 1624.53 1635.64
1655.26 1657.05 3006.11 3031.51 3070.61 3163.63
3168.97 3169.86 3176.51 3181.76 3189.60 3193.73
3195.17 3199.41 3201.79 3289.05 3290.18 3290.54
3318.21 3319.31 3319.70 3622.22 3678.31 3681.64

³2 (R=H)

13.10 24.22 31.05 44.28 58.30 58.83
70.32 74.36 78.34 114.60 147.64 151.50
164.23 169.95 179.37 192.36 195.63 207.22
224.72 244.32 255.69 285.34 302.54 308.44
331.25 336.75 344.54 352.59 359.82 370.01
403.55 418.90 423.92 476.95 505.79 565.10
581.01 590.34 601.50 612.37 633.22 633.44
637.11 641.42 653.86 661.94 689.40 697.88
705.60 715.71 719.99 727.47 729.86 733.21
748.70 763.79 775.19 791.37 819.41 834.66
838.65 845.09 864.65 884.74 894.64 900.59
924.99 940.81 941.16 943.33 946.20 953.57
971.70 995.08 995.18 1000.51 1000.99 1004.42
1007.47 1014.26 1015.79 1018.22 1051.73 1055.21
1064.24 1089.24 1098.13 1100.91 1103.84 1104.44
1107.57 1123.47 1125.52 1134.43 1137.95 1184.67
1188.70 1198.18 1198.97 1203.28 1215.27 1221.34
1223.60 1231.14 1234.54 1242.04 1255.95 1272.56
1288.15 1294.46 1319.56 1322.59 1336.58 1361.71
1369.04 1412.56 1413.32 1416.08 1428.85 1463.74
1469.06 1473.48 1478.98 1493.47 1509.65 1536.42
1537.95 1603.80 1606.71 1609.92 1625.34 1637.31
1656.67 1659.98 3015.91 3047.08 3104.72 3159.40
3168.45 3172.37 3176.06 3181.93 3188.52 3193.98
3195.39 3200.94 3201.97 3288.64 3288.78 3292.03
3313.76 3314.40 3314.59 3659.87 3680.83 3682.80

¹2 (R=H)

22.07 30.41 35.74 43.00 58.63 64.68
68.31 74.77 82.39 112.15 143.54 166.28
175.60 184.93 198.96 201.73 206.78 213.65
234.15 247.91 251.20 319.30 334.05 338.76

351.10 365.21 373.09 378.66 381.68 390.73
420.80 422.57 425.07 481.59 503.92 550.71
580.53 591.52 595.78 608.85 632.85 634.26
636.08 645.38 657.59 668.33 687.98 699.31
700.57 713.56 719.22 723.94 736.03 740.99
758.81 765.84 777.69 799.09 818.20 831.50
833.21 834.14 839.75 862.82 883.10 897.00
921.88 941.09 941.85 945.51 951.03 953.54
969.10 990.49 994.72 1004.06 1004.81 1010.90
1014.06 1014.37 1018.18 1027.74 1053.22 1058.54
1064.86 1100.54 1101.32 1101.98 1105.25 1106.82
1108.79 1123.85 1128.45 1134.55 1140.08 1185.12
1187.03 1198.38 1205.16 1213.35 1218.02 1221.13
1222.48 1224.84 1227.59 1241.22 1256.64 1283.30
1286.66 1299.46 1319.14 1331.21 1332.83 1364.34
1367.85 1406.94 1416.77 1420.13 1440.05 1460.93
1468.67 1472.04 1479.74 1493.45 1517.33 1537.59
1537.68 1601.75 1603.79 1607.94 1623.70 1635.94
1655.21 1657.20 3026.22 3076.25 3094.60 3166.92
3167.74 3172.05 3175.25 3185.35 3189.17 3194.65
3198.12 3201.00 3203.34 3286.72 3289.07 3289.56
3307.89 3314.04 3314.40 3627.41 3679.48 3685.01

³1''-TS (R=H)

-665.68 18.39 28.44 38.55 43.85 53.27
58.37 62.84 68.28 75.97 86.25 102.40
130.67 145.89 155.78 166.45 168.64 181.95
187.74 192.74 198.08 229.19 243.32 258.17
267.82 270.16 291.99 296.52 307.13 315.09
336.87 342.54 352.48 356.43 360.65 418.53
420.27 461.67 502.79 524.87 601.72 604.34
608.90 609.83 621.33 625.25 642.34 644.18
651.74 656.97 662.92 671.26 684.30 694.71
704.01 705.31 720.42 722.87 725.13 727.49
745.65 764.77 785.73 801.38 813.70 825.12
838.93 846.07 847.90 877.50 891.12 908.43
931.49 932.35 935.55 940.52 957.95 960.23
980.98 982.40 990.88 995.40 1000.56 1001.98
1004.90 1011.59 1017.29 1041.56 1056.81 1063.97
1074.95 1094.61 1096.59 1103.43 1104.70 1106.53
1116.24 1120.09 1123.74 1159.39 1162.26 1191.08
1196.95 1200.46 1201.90 1207.37 1209.38 1226.34
1238.06 1246.43 1259.33 1263.96 1292.67 1308.45
1321.93 1329.60 1330.77 1360.10 1366.26 1374.39
1403.37 1412.65 1418.22 1431.47 1440.77 1450.86
1454.69 1462.63 1471.59 1473.73 1474.86 1520.63
1526.42 1553.79 1606.87 1610.00 1613.19 1637.63
1646.94 1671.59 1672.10 2935.05 3058.73 3114.08
3133.66 3155.23 3156.74 3156.94 3161.10 3166.93
3170.54 3174.65 3176.54 3188.92 3189.07 3221.33
3263.91 3269.45 3269.70 3288.26 3291.38 3291.64
3622.29 3664.79 3686.73

³1'-TS (R=H)

-557.69 12.52 21.88 25.89 43.66 52.50
54.58 60.07 66.83 80.24 93.62 102.50
122.59 139.98 140.89 157.36 170.18 173.56
185.11 188.43 189.88 216.76 233.50 256.97
262.02 273.25 293.09 304.71 315.86 319.92
338.82 345.19 351.79 363.72 381.53 409.29
416.52 417.93 501.31 507.00 583.38 588.98
604.43 611.38 618.52 620.09 626.74 633.87
645.12 648.99 677.08 686.42 691.67 700.52
715.27 717.83 722.29 726.10 735.59 743.36
744.27 789.07 790.67 812.79 833.44 833.98
836.86 837.84 840.89 876.75 892.04 895.40
931.05 932.21 935.92 940.12 941.75 951.40
968.77 975.15 982.30 994.21 995.47 998.86

1001.00 1003.40 1013.13 1026.98 1052.57 1064.37
1091.63 1093.32 1098.75 1102.87 1103.31 1117.83
1119.47 1123.23 1124.60 1155.79 1162.74 1184.01
1200.13 1203.56 1207.90 1211.62 1224.58 1227.73
1236.36 1254.39 1270.19 1272.52 1295.78 1310.22
1313.75 1322.68 1333.19 1333.55 1361.90 1375.69
1390.37 1405.68 1410.92 1429.74 1450.28 1453.84
1458.16 1459.72 1464.64 1465.42 1475.84 1520.38
1527.19 1580.06 1606.81 1608.16 1612.67 1629.60
1640.18 1658.57 1673.29 3017.07 3088.02 3105.08
3137.61 3146.73 3153.50 3157.33 3160.90 3160.97
3169.94 3173.12 3176.68 3180.09 3187.84 3190.53
3260.31 3268.84 3270.15 3284.31 3290.91 3292.13
3587.10 3676.62 3687.04

⁵1a (p-NO₂)

13.32 22.68 29.94 31.58 42.69 54.44
63.63 65.75 74.66 78.46 94.50 97.90
137.53 144.31 157.62 161.18 166.25 180.37
191.44 194.55 199.29 227.66 251.34 260.66
273.38 277.38 297.03 301.42 316.30 331.07
333.88 345.33 353.20 362.21 409.51 424.91
436.70 471.88 493.28 507.24 530.44 544.14
604.00 612.98 615.50 628.16 635.64 639.54
649.59 653.46 663.88 676.34 685.41 700.24
709.52 710.64 728.35 730.85 735.87 739.75
742.04 753.71 766.76 793.79 796.01 822.85
833.65 840.01 845.76 854.01 855.29 858.23
887.17 895.79 934.89 942.52 943.50 946.35
954.63 982.64 992.05 996.62 1003.75 1006.02
1009.92 1010.35 1015.93 1018.20 1053.17 1065.13
1082.34 1105.16 1108.33 1109.35 1110.30 1127.75
1128.27 1130.61 1132.10 1137.97 1189.43 1194.92
1199.51 1205.79 1212.57 1213.37 1224.17 1232.29
1242.87 1253.70 1261.21 1267.05 1289.28 1299.84
1305.08 1319.68 1325.99 1329.20 1358.89 1370.08
1373.08 1417.42 1418.25 1432.95 1445.62 1455.41
1459.09 1464.53 1473.16 1479.40 1483.14 1527.85
1538.40 1557.65 1601.93 1605.98 1613.47 1618.84
1625.27 1627.57 1656.16 2966.76 2996.36 3163.34
3170.15 3177.35 3189.77 3192.53 3194.96 3202.15
3210.29 3239.04 3242.30 3290.33 3292.73 3293.59
3317.70 3318.49 3319.79 3618.28 3675.80 3680.59

³1a (p-NO₂)

14.79 23.98 33.79 42.47 47.76 51.62
66.83 67.43 80.16 85.38 90.06 109.94
159.71 167.37 173.65 174.99 180.29 193.13
199.01 225.33 231.90 251.86 262.88 281.29
293.58 306.01 327.91 334.57 345.32 348.97
359.27 368.75 380.11 394.44 423.87 425.54
454.63 482.57 504.70 523.30 549.08 606.48
609.03 614.19 619.66 631.02 635.41 636.06
650.38 655.97 661.57 676.81 688.13 698.12
708.81 711.25 726.76 729.20 735.27 741.02
743.67 756.27 772.61 790.21 798.70 823.15
828.12 833.47 844.64 852.47 855.53 857.29
885.56 898.55 943.02 944.80 947.71 953.50
973.34 982.63 991.46 995.26 1006.07 1010.93
1012.30 1013.63 1018.39 1026.03 1057.91 1064.82
1098.02 1103.91 1105.11 1107.76 1109.51 1127.04
1127.48 1132.13 1136.93 1137.88 1188.95 1200.85
1202.44 1211.94 1214.20 1222.03 1224.44 1238.51
1241.89 1244.31 1265.71 1267.78 1298.14 1306.67
1318.08 1320.92 1330.25 1334.52 1360.31 1368.82
1372.43 1422.70 1425.47 1443.91 1444.02 1457.24
1462.76 1472.14 1473.45 1478.94 1487.59 1524.98
1537.78 1561.70 1596.92 1601.09 1608.49 1618.82

1623.45 1632.26 1654.82 2991.27 3028.11 3164.69
3169.65 3176.86 3184.16 3188.77 3194.44 3201.60
3219.99 3239.63 3241.45 3291.79 3292.43 3293.26
3315.44 3315.57 3315.98 3646.53 3677.38 3679.40

¹a (p-NO₂)

10.39 23.78 29.52 30.87 42.64 52.93
63.87 67.37 76.63 89.12 93.60 110.76
156.80 170.95 173.99 177.03 185.98 193.73
199.71 225.88 230.63 246.44 256.34 279.26
289.88 320.27 327.69 337.46 340.24 349.63
365.42 371.89 391.88 399.34 424.07 425.35
458.16 478.54 504.43 528.28 552.84 604.12
612.47 619.55 626.19 635.84 636.19 642.17
650.40 654.93 659.79 684.13 687.87 699.62
708.74 712.04 726.71 728.57 736.11 739.81
743.66 754.13 772.41 792.70 800.11 821.10
831.25 837.59 842.78 850.08 857.39 860.33
885.15 899.67 943.52 944.78 948.24 953.30
975.62 982.89 992.19 995.76 1006.16 1011.38
1012.23 1015.13 1018.58 1028.64 1065.29 1068.29
1103.88 1108.15 1108.41 1109.76 1117.49 1127.34
1130.50 1131.71 1137.19 1139.59 1189.19 1201.13
1204.67 1211.73 1215.94 1222.68 1224.90 1236.13
1242.84 1245.19 1265.71 1269.31 1297.83 1311.73
1318.59 1322.84 1330.78 1338.51 1360.73 1369.21
1375.46 1424.47 1426.32 1445.00 1445.65 1456.86
1464.67 1473.19 1476.13 1479.16 1491.68 1527.98
1538.57 1562.53 1598.89 1601.68 1607.82 1618.97
1625.20 1631.11 1656.38 2983.31 3012.43 3170.08
3170.80 3177.49 3189.66 3193.89 3195.20 3202.13
3213.44 3240.41 3242.31 3290.78 3292.62 3292.83
3313.62 3315.64 3316.86 3629.39 3674.70 3685.28

⁵a (p-NMe₂)

19.41 25.41 30.22 36.76 47.91 62.81
65.48 68.80 78.86 93.94 95.00 108.07
132.06 136.96 149.34 164.52 165.93 179.67
188.51 189.81 193.81 206.80 232.18 252.14
259.97 264.59 288.55 293.65 300.75 319.94
328.06 338.30 346.40 349.16 351.36 361.65
365.08 408.08 425.51 431.36 471.94 500.22
507.74 515.03 538.68 553.28 598.26 610.47
618.73 635.28 646.26 647.13 652.04 662.55
669.33 685.32 694.56 697.51 707.85 708.62
724.01 728.83 731.48 734.58 744.13 751.63
797.46 802.41 812.43 821.62 827.43 833.28
840.10 847.51 884.78 893.40 928.26 936.09
942.12 943.06 945.54 946.13 952.28 959.33
995.92 1001.17 1004.31 1006.33 1007.66 1014.83
1016.59 1041.36 1062.13 1063.91 1096.76 1103.96
1106.79 1107.93 1110.17 1124.17 1127.29 1135.33
1152.89 1160.40 1162.65 1188.17 1195.47 1201.22
1205.03 1207.77 1212.83 1213.66 1223.16 1231.16
1240.34 1250.26 1255.56 1263.98 1265.82 1282.88
1293.53 1310.63 1318.51 1320.94 1343.62 1358.37
1369.20 1391.83 1415.71 1417.91 1431.38 1432.14
1450.96 1457.86 1464.24 1465.97 1472.79 1479.41
1488.41 1496.74 1503.72 1506.71 1534.71 1537.41
1539.19 1551.92 1561.17 1602.49 1606.20 1610.80
1624.93 1638.52 1655.36 2887.68 2895.53 2937.64
2967.19 2968.28 2974.92 3095.85 3109.12 3153.54
3167.99 3175.81 3176.55 3189.23 3195.15 3198.03
3201.28 3217.25 3218.75 3287.67 3289.58 3290.07
3315.43 3316.45 3317.58 3592.98 3675.93 3682.59

³a (p-NMe₂)

17.33 18.22 28.71 37.50 43.60 48.10
63.79 69.08 75.11 79.67 90.73 110.32
140.69 148.40 159.65 168.69 178.51 179.65
195.16 198.84 201.85 217.90 229.80 243.01
254.36 268.99 278.43 319.46 323.82 338.59
343.99 350.38 355.18 374.40 375.53 391.14
403.51 420.60 423.09 442.53 482.37 504.89
511.34 530.05 563.34 601.46 610.69 611.93
622.30 635.60 646.18 646.93 653.00 655.65
660.77 683.64 694.72 698.83 703.30 708.58
722.74 727.35 732.86 735.14 736.66 757.23
797.58 801.10 802.06 823.22 824.30 824.57
838.47 846.57 883.67 898.36 934.32 941.29
943.74 944.22 948.28 952.33 959.50 976.10
994.17 1004.18 1008.41 1009.24 1013.52 1016.92
1026.70 1045.44 1064.98 1085.00 1102.46 1104.12
1106.59 1108.40 1127.92 1128.68 1132.03 1137.68
1138.24 1150.84 1160.35 1188.33 1197.92 1199.65
1205.84 1213.37 1217.33 1221.90 1224.46 1231.27
1241.45 1242.34 1261.31 1266.79 1268.86 1288.53
1305.48 1319.85 1324.85 1334.53 1352.43 1362.78
1368.43 1382.98 1421.95 1425.06 1431.11 1444.29
1454.52 1456.72 1461.11 1472.59 1473.44 1473.95
1488.00 1495.31 1497.15 1502.51 1524.32 1535.58
1537.98 1546.58 1567.79 1598.98 1602.25 1607.59
1624.83 1640.87 1655.74 2938.60 2980.25 2988.72
3001.29 3075.11 3076.87 3127.43 3137.60 3143.34
3162.27 3166.63 3174.76 3187.79 3193.81 3200.01
3212.85 3218.41 3232.42 3287.97 3289.01 3290.76
3312.88 3313.41 3313.56 3653.60 3676.41 3679.48

¹a (p-NMe₂)

18.21 25.44 29.69 34.82 43.23 63.50
66.40 68.79 79.25 99.59 107.57 111.00
151.84 156.19 170.95 173.36 180.71 195.24
199.61 204.75 224.55 229.11 245.83 250.94
259.00 283.07 319.87 323.36 339.88 346.03
350.01 357.80 373.44 375.46 389.86 396.34
419.89 423.50 444.71 458.28 485.37 505.42
514.67 541.65 563.77 603.67 613.71 621.64
633.74 635.70 649.93 650.41 655.45 660.04
686.06 692.71 698.75 705.48 707.66 709.38
724.31 727.19 736.20 739.60 745.91 760.62
801.10 807.69 813.27 824.10 826.80 828.64
837.81 847.44 883.85 898.44 928.73 943.39
944.39 947.46 949.02 952.04 961.37 975.27
994.80 1004.38 1005.75 1009.59 1013.90 1017.30
1028.03 1064.71 1070.72 1102.94 1104.78 1106.88
1108.53 1109.88 1128.97 1130.56 1135.68 1146.20
1148.81 1155.91 1187.62 1192.56 1200.00 1202.18
1211.07 1215.52 1218.70 1222.54 1225.45 1234.23
1241.32 1244.88 1261.27 1267.33 1277.33 1292.41
1303.60 1318.53 1321.03 1331.03 1344.65 1365.48
1368.31 1395.86 1423.29 1424.78 1438.97 1443.46
1455.02 1462.80 1469.21 1472.17 1475.81 1481.18
1491.18 1500.72 1511.69 1515.73 1532.05 1538.01
1541.10 1552.29 1562.07 1598.51 1602.25 1608.71
1623.81 1641.26 1655.51 2817.71 2869.57 2932.42
2946.72 2963.29 3001.49 3055.46 3118.77 3159.02
3167.83 3173.77 3175.24 3187.23 3189.47 3194.82
3201.14 3211.30 3214.72 3288.64 3290.38 3290.51
3311.71 3313.77 3314.94 3610.66 3675.86 3684.68

⁵1-TS (p-NO₂)

-322.29 21.77 25.21 30.76 45.98 50.21
65.13 66.50 69.98 77.21 89.74 96.62
104.22 118.70 137.43 146.13 166.49 171.99
185.51 189.68 193.59 217.14 234.06 243.23

247.96 262.14 270.42 290.83 298.89 316.94
323.44 337.86 345.60 351.22 353.45 369.73
425.79 434.82 483.02 500.22 508.07 554.89
612.61 620.84 626.20 628.52 635.11 635.57
653.52 656.28 661.41 668.94 689.43 697.60
711.36 729.79 731.72 732.71 735.48 741.77
744.61 753.49 778.86 781.09 791.87 798.29
824.71 833.87 845.61 850.47 852.68 853.75
866.88 886.52 894.45 938.00 939.73 943.64
945.26 954.09 962.69 983.93 985.42 996.38
1004.18 1004.49 1008.84 1014.31 1015.49 1018.64
1044.30 1063.91 1105.65 1108.97 1110.09 1119.72
1130.45 1131.64 1136.64 1139.18 1142.79 1188.52
1195.68 1202.81 1210.90 1213.28 1223.21 1231.07
1243.20 1249.78 1250.66 1263.83 1293.76 1296.28
1301.20 1319.19 1323.50 1333.11 1360.86 1368.81
1382.54 1419.13 1423.52 1436.08 1447.91 1459.59
1463.07 1468.26 1471.85 1474.51 1526.69 1537.51
1572.93 1599.23 1602.70 1603.65 1613.66 1623.49
1632.39 1646.64 1654.14 3168.38 3169.91 3176.61
3187.49 3188.53 3189.83 3193.58 3201.60 3216.14
3232.66 3233.45 3272.27 3291.17 3291.92 3297.56
3317.44 3317.70 3323.38 3601.53 3670.42 3675.26

³¹1-TS (p-NO₂)

-270.27 11.89 23.11 31.49 34.54 43.83
54.50 65.90 67.03 78.50 90.34 102.99
109.05 155.25 165.00 169.03 174.40 178.32
193.64 197.96 209.67 218.38 240.06 256.09
270.83 297.60 308.47 325.31 328.59 336.68
345.06 361.63 361.97 376.08 389.17 421.52
424.52 432.25 491.32 504.15 506.79 544.34
608.33 615.37 623.19 628.90 635.72 640.91
651.63 654.53 661.50 687.17 693.05 706.80
712.51 717.98 729.19 731.47 736.53 738.80
747.45 755.57 780.51 788.12 798.53 822.69
840.89 842.42 847.06 854.91 862.21 869.49
885.84 886.85 898.94 942.25 944.44 945.51
947.95 954.97 983.30 993.09 995.88 1006.84
1009.50 1014.53 1018.16 1018.68 1028.92 1061.46
1065.59 1086.40 1104.90 1108.96 1109.97 1112.91
1131.77 1133.14 1134.07 1138.18 1140.38 1190.03
1203.40 1212.95 1213.84 1221.26 1225.22 1239.83
1245.49 1246.93 1258.67 1278.50 1292.14 1296.29
1311.38 1321.04 1329.64 1336.10 1360.82 1369.73
1375.15 1422.00 1426.74 1442.22 1449.59 1462.23
1471.46 1472.52 1473.71 1487.23 1525.07 1538.63
1565.26 1586.29 1601.35 1604.41 1611.01 1625.03
1636.48 1642.52 1655.90 3158.13 3169.41 3170.85
3178.05 3187.06 3189.77 3195.42 3202.45 3203.76
3237.14 3240.15 3250.61 3292.23 3295.33 3297.45
3316.80 3318.37 3319.35 3590.43 3675.20 3685.19

¹1-TS (CSS) (p-NO₂)

-478.37 9.89 23.30 25.42 36.24 45.42
55.11 64.43 70.11 71.00 88.38 91.64
113.55 148.93 160.08 174.61 183.99 186.71
196.90 207.96 217.90 229.98 239.11 254.14
271.08 290.26 312.09 321.55 334.08 342.95
359.87 364.15 376.59 388.64 402.22 426.60
430.96 450.35 495.68 505.24 508.66 542.05
572.48 592.59 596.54 626.77 629.80 632.01
634.89 639.12 641.02 649.95 685.81 691.60
698.60 702.91 717.92 723.35 728.53 736.57
743.26 757.09 775.94 785.84 789.68 816.44
825.39 832.51 834.49 839.24 845.24 850.47
871.29 885.39 890.21 942.81 943.57 946.37
953.20 955.02 983.31 988.64 997.82 1004.46

1006.15 1008.59 1014.81 1015.96 1022.17 1062.41
1068.04 1098.89 1099.25 1102.90 1108.08 1126.04
1130.18 1131.27 1133.65 1139.67 1142.56 1189.69
1200.40 1207.33 1212.42 1214.59 1224.13 1234.56
1237.98 1241.58 1248.98 1264.19 1280.63 1286.01
1300.58 1318.64 1327.04 1331.92 1368.66 1369.70
1377.25 1414.51 1418.78 1433.13 1443.98 1469.61
1471.19 1476.50 1479.92 1489.77 1522.89 1537.37
1564.52 1588.27 1606.14 1606.70 1610.50 1624.43
1640.51 1644.17 1655.95 3155.53 3170.41 3174.88
3178.00 3185.47 3190.24 3196.18 3202.53 3225.23
3234.23 3240.31 3242.65 3292.83 3293.97 3294.65
3315.65 3318.14 3318.54 3674.78 3686.51 3690.03

¹¹1-TS (OSS) (p-NO₂)

-719.69 10.63 22.99 26.46 36.23 47.28
55.00 65.12 69.88 70.98 87.49 88.53
111.82 134.64 156.78 173.11 178.53 183.23
193.40 195.69 205.51 219.20 238.34 251.27
255.73 289.82 309.79 310.68 328.79 338.83
352.86 358.43 367.60 376.77 386.82 420.31
426.74 431.40 492.71 499.26 506.28 540.44
577.06 593.16 595.13 623.93 630.83 632.48
634.61 638.37 641.27 649.77 686.09 686.59
697.60 703.98 718.36 723.67 725.56 733.42
736.62 749.41 757.44 773.58 788.22 790.43
816.87 836.38 836.95 839.51 845.66 847.32
872.35 885.35 890.25 943.03 943.30 944.05
946.70 954.94 985.02 990.20 997.87 1004.20
1006.13 1008.14 1014.54 1015.43 1020.26 1060.00
1062.18 1076.39 1099.17 1099.79 1103.17 1107.87
1124.41 1129.55 1131.25 1137.41 1141.27 1189.52
1199.21 1206.66 1210.86 1213.98 1224.07 1233.51
1233.91 1238.65 1249.21 1263.36 1279.58 1285.65
1300.35 1318.76 1326.27 1331.85 1367.30 1369.67
1376.41 1413.99 1417.94 1432.32 1440.69 1467.28
1470.89 1475.73 1478.63 1486.55 1523.00 1537.33
1560.39 1588.60 1605.52 1606.42 1610.02 1624.52
1637.13 1645.36 1655.97 3162.38 3167.53 3170.81
3178.34 3185.00 3190.58 3196.53 3202.93 3223.19
3240.95 3241.84 3245.79 3293.35 3293.97 3295.39
3316.54 3318.38 3319.84 3681.10 3685.52 3687.38

⁵¹1-TS (p-NMe₂)

-396.40 15.57 22.16 27.26 29.94 40.98
42.08 60.99 65.08 69.09 71.67 88.87
89.28 115.80 128.71 131.72 149.75 162.67
164.58 172.76 185.06 193.54 198.63 211.66
222.72 230.95 241.17 261.64 262.35 278.56
297.45 301.66 317.57 320.29 345.85 349.31
359.98 364.62 390.22 422.44 425.28 460.18
491.22 507.82 522.38 547.16 611.90 619.75
623.45 635.75 650.45 653.33 656.23 671.54
675.11 681.73 691.34 694.73 700.23 711.61
719.90 729.33 732.06 735.64 742.88 752.23
753.91 798.03 814.74 819.96 823.30 838.24
840.18 842.95 850.07 885.96 893.24 933.56
937.52 942.56 943.06 945.08 946.02 953.63
957.06 965.12 996.29 1002.33 1003.15 1008.04
1012.48 1016.81 1018.65 1052.12 1064.37 1083.93
1105.22 1108.49 1108.84 1114.40 1128.47 1130.00
1135.28 1138.44 1152.89 1160.55 1188.47 1195.11
1197.48 1202.34 1209.32 1217.15 1222.52 1229.63
1248.76 1249.21 1258.45 1268.52 1269.98 1286.88
1293.85 1302.72 1318.48 1319.29 1348.98 1362.92
1369.35 1374.15 1419.78 1420.44 1434.15 1442.68
1456.30 1459.14 1460.88 1472.73 1474.32 1476.27
1496.32 1498.03 1503.63 1524.43 1537.71 1540.67

1558.03 1580.14 1600.19 1603.38 1607.08 1608.25
1625.05 1655.51 1661.98 2979.29 2988.96 3073.29
3076.01 3127.44 3137.41 3149.35 3168.51 3173.05
3176.21 3183.91 3188.67 3194.35 3195.68 3200.99
3218.92 3223.45 3268.57 3288.69 3289.51 3290.97
3315.90 3316.37 3318.39 3591.03 3672.79 3673.30

³¹I-TS (p-NMe₂)

-423.45 12.19 19.54 25.39 34.23 43.42
49.19 62.87 65.74 72.78 82.56 92.52
108.62 144.64 154.59 156.27 166.63 173.58
173.72 189.82 195.04 199.14 211.15 222.05
239.00 242.21 256.39 302.33 309.24 314.88
327.51 335.77 345.82 353.54 361.88 371.18
381.57 399.72 421.88 426.84 443.74 462.04
494.32 507.26 531.73 541.73 606.51 613.10
622.10 632.63 648.93 650.06 651.13 660.39
682.93 690.69 699.09 707.54 709.35 709.97
725.65 728.19 735.59 739.32 755.12 758.14
794.00 798.56 818.64 820.55 823.20 830.32
837.71 841.98 850.00 884.74 890.17 934.04
941.15 942.90 944.92 946.88 947.40 953.37
966.01 997.19 1004.39 1005.37 1009.33 1015.87
1017.18 1025.90 1062.41 1064.64 1073.79 1084.99
1103.65 1107.79 1108.03 1112.45 1128.29 1130.73
1136.34 1138.89 1152.23 1159.89 1188.16 1197.54
1198.02 1212.87 1215.01 1221.79 1224.38 1239.93
1242.18 1245.36 1254.01 1269.39 1276.66 1286.32
1291.93 1304.24 1318.62 1329.20 1342.64 1363.64
1368.96 1376.18 1421.65 1425.38 1438.89 1441.53
1457.21 1459.70 1467.44 1471.11 1475.59 1487.26
1495.20 1497.56 1502.22 1523.94 1536.80 1540.05
1551.24 1558.26 1590.35 1599.93 1603.35 1609.92
1622.96 1654.20 1659.71 2964.73 2976.99 3073.02
3074.57 3126.94 3136.64 3147.29 3154.71 3168.95
3173.57 3176.30 3189.63 3191.71 3195.14 3201.70
3218.86 3220.43 3235.27 3290.24 3292.38 3294.26
3314.71 3314.89 3316.38 3583.48 3676.27 3683.42

¹¹I-TS (CSS) (p-NMe₂)

-487.67 16.54 21.88 30.01 36.35 44.61
48.95 66.69 69.07 73.15 83.17 89.77
113.06 131.01 161.46 166.26 176.08 182.07
186.19 197.73 199.97 206.74 220.64 231.58
247.02 256.41 262.03 295.98 307.59 315.20
331.47 340.47 354.70 362.11 378.53 390.12
395.47 422.42 426.23 436.60 457.63 463.97
493.35 508.01 531.32 546.67 565.31 584.55
601.05 629.47 635.79 636.32 643.80 648.46
653.04 680.74 693.12 694.70 696.74 711.45
719.11 722.23 725.72 735.77 756.27 766.05
788.03 796.24 801.76 811.56 816.83 822.46
830.58 836.73 841.83 883.57 894.65 941.82
942.11 943.88 945.30 948.60 951.86 957.87
966.76 995.85 1003.21 1005.05 1010.59 1011.60
1016.12 1021.48 1064.45 1067.52 1085.95 1097.54
1098.60 1101.43 1106.13 1109.96 1125.47 1127.47
1138.62 1141.16 1148.84 1163.50 1187.79 1197.33
1199.38 1206.12 1214.98 1216.39 1222.68 1229.51
1235.86 1239.70 1255.30 1257.35 1271.82 1275.32
1290.28 1291.77 1317.95 1318.81 1353.71 1368.26
1372.84 1386.68 1412.59 1416.54 1431.44 1448.82
1460.34 1468.20 1473.47 1474.15 1481.08 1484.59
1495.59 1497.87 1503.20 1525.28 1537.36 1540.67
1555.44 1574.68 1596.53 1606.02 1606.40 1610.32
1624.66 1655.34 1661.44 2978.56 3001.09 3073.51
3074.70 3132.49 3143.24 3150.22 3162.33 3165.94
3170.51 3174.41 3188.13 3194.85 3200.52 3212.10

3223.26 3227.30 3230.20 3288.39 3288.75 3288.87
3309.91 3314.00 3314.26 3657.07 3687.88 3692.16

¹¹I-TS (OSS) (p-NMe₂)

-741.56 16.94 23.04 27.83 34.16 44.45
47.49 67.51 69.52 72.19 81.53 89.14
112.75 128.73 159.31 161.62 174.68 177.02
182.62 195.98 201.05 204.53 214.71 219.98
228.81 250.54 257.04 284.49 300.31 312.82
325.31 334.07 352.14 358.53 373.24 382.31
390.19 406.12 425.30 431.18 433.97 461.05
492.09 506.48 529.66 543.91 570.35 587.02
599.35 631.08 634.79 637.25 641.53 643.32
652.12 681.64 690.39 693.22 698.21 711.74
712.42 715.13 722.82 728.11 735.65 755.81
770.81 788.23 792.37 811.13 816.49 823.45
831.33 837.67 838.32 883.81 895.56 939.82
942.22 942.92 945.59 949.92 951.28 952.37
963.11 995.99 1003.10 1005.00 1010.05 1010.29
1015.83 1020.02 1061.71 1064.29 1076.07 1085.64
1097.77 1099.30 1101.54 1106.41 1126.18 1127.79
1138.99 1140.82 1149.25 1162.00 1188.15 1197.12
1197.90 1205.26 1213.61 1214.37 1223.23 1232.48
1235.07 1242.12 1249.42 1258.53 1272.39 1273.75
1285.69 1291.07 1317.86 1318.58 1350.73 1368.54
1370.17 1384.46 1412.44 1415.95 1430.67 1443.98
1458.18 1469.60 1474.14 1475.71 1479.40 1484.66
1495.45 1497.40 1502.91 1525.06 1537.53 1540.51
1552.40 1565.69 1591.91 1605.75 1606.58 1610.35
1624.80 1655.41 1658.19 2975.46 3000.50 3073.60
3074.72 3131.04 3141.98 3152.78 3158.08 3166.40
3168.51 3174.84 3188.44 3195.07 3201.48 3207.28
3222.00 3226.46 3236.68 3289.60 3289.78 3289.83
3311.26 3314.55 3316.08 3665.35 3687.73 3691.16

³¹Ia-TS (p-NO₂)

-336.52 15.05 24.14 33.19 41.88 44.40
55.64 65.96 67.47 78.74 91.91 99.63
111.28 151.56 172.43 174.63 176.30 185.97
193.94 197.42 220.23 236.16 253.55 257.43
280.59 306.47 312.21 322.57 334.61 345.13
346.44 357.08 369.67 375.46 379.73 426.30
430.33 483.46 498.03 506.12 533.88 543.41
594.05 602.12 616.78 631.42 632.91 641.41
643.55 647.89 653.95 677.15 694.31 696.78
707.01 709.77 723.83 725.72 736.13 736.65
740.17 754.43 763.86 791.18 794.58 818.59
830.26 838.99 843.08 849.37 854.78 861.83
885.96 894.43 942.87 943.86 946.59 954.60
981.76 989.39 997.42 1004.43 1005.76 1006.47
1010.20 1013.90 1017.03 1020.69 1063.41 1072.59
1101.84 1105.59 1106.63 1109.22 1129.50 1131.22
1133.16 1136.30 1140.58 1163.22 1189.47 1201.25
1202.83 1209.35 1215.24 1216.37 1224.34 1235.71
1242.52 1250.97 1263.48 1267.10 1290.19 1297.30
1304.39 1320.53 1327.78 1330.84 1358.20 1370.06
1372.27 1417.17 1419.83 1435.09 1443.97 1467.57
1473.07 1473.51 1479.47 1483.24 1499.93 1534.31
1538.10 1563.42 1603.20 1605.66 1608.90 1625.17
1627.81 1633.37 1656.31 2991.79 3030.35 3171.38
3178.56 3182.98 3190.60 3196.23 3203.27 3207.04
3213.61 3237.85 3238.82 3294.07 3294.13 3294.60
3317.47 3319.38 3320.56 3626.91 3680.88 3687.77

¹¹Ia-TS (p-NO₂)

-557.65 17.59 20.23 31.75 40.77 47.41
62.06 65.34 67.55 76.73 104.29 112.07

142.40 161.43 171.14 174.63 179.25 195.82
 199.87 222.41 233.11 246.56 259.17 270.89
 287.70 318.58 321.08 339.88 343.24 347.36
 362.89 374.43 392.56 411.09 423.51 429.15
 441.87 482.78 503.84 506.01 543.45 591.28
 603.43 611.35 620.70 630.31 633.77 641.69
 650.27 654.73 658.54 685.41 691.42 700.11
 709.84 713.21 726.07 728.42 734.86 736.54
 744.32 755.20 764.80 789.14 798.73 820.38
 834.41 839.14 841.17 848.90 854.86 860.86
 885.49 899.56 943.22 944.79 947.32 953.78
 981.45 992.09 995.65 998.81 1006.79 1011.75
 1013.02 1014.05 1018.83 1028.95 1064.62 1073.60
 1102.32 1107.45 1108.17 1109.78 1129.00 1131.25
 1132.60 1138.35 1139.17 1161.53 1189.18 1194.77
 1205.57 1212.73 1216.41 1223.12 1225.07 1237.82
 1242.60 1245.53 1263.53 1269.46 1296.86 1299.17
 1311.53 1322.52 1328.84 1336.66 1356.79 1369.28
 1374.00 1424.18 1425.35 1443.22 1444.80 1458.38
 1470.27 1473.60 1476.15 1479.56 1498.99 1530.32
 1538.59 1562.11 1598.42 1602.63 1607.29 1624.59
 1624.80 1628.15 1656.84 2973.59 3007.73 3169.30
 3176.24 3188.05 3188.64 3193.53 3193.94 3201.30
 3209.15 3236.27 3239.91 3290.87 3291.94 3294.56
 3313.72 3316.70 3317.31 3609.71 3673.89 3682.19

³1a-TS (p-NMe₂)

 -427.76 17.33 22.38 33.71 41.33 43.73
 54.16 65.23 66.58 79.08 84.07 92.88
 110.55 143.26 147.91 163.52 170.30 175.32
 191.39 194.10 194.94 206.36 217.09 227.96
 251.09 255.13 261.32 297.46 314.83 319.82
 332.20 340.89 347.58 351.51 361.45 370.65
 376.23 404.67 422.56 424.89 450.55 487.21
 506.56 519.82 520.95 549.06 584.86 593.64
 615.67 633.09 638.18 645.62 646.38 654.30
 677.03 684.43 690.10 699.62 700.69 708.34
 716.88 723.13 731.70 734.66 735.75 752.84
 794.12 812.40 815.48 817.45 827.52 829.97
 834.25 840.50 884.25 894.09 936.42 941.21
 941.56 942.54 945.52 952.33 963.17 995.20
 1001.56 1003.31 1005.06 1009.37 1015.43 1016.45
 1017.17 1064.04 1082.42 1085.61 1098.42 1103.01
 1104.42 1107.52 1124.36 1127.41 1135.92 1138.64
 1149.64 1151.27 1170.19 1188.16 1192.34 1197.50
 1200.90 1207.94 1215.72 1220.20 1223.74 1235.34
 1236.91 1242.09 1259.35 1261.96 1271.19 1279.61
 1290.94 1297.52 1317.76 1320.80 1344.58 1363.57
 1368.99 1378.27 1413.96 1416.50 1432.07 1433.76
 1457.41 1467.38 1469.26 1472.94 1477.49 1481.90
 1495.22 1497.30 1501.25 1504.56 1524.64 1537.90
 1539.95 1552.40 1577.09 1604.25 1605.61 1609.64
 1624.55 1650.63 1655.88 2968.28 2972.10 2981.47
 3004.98 3073.67 3075.53 3128.81 3138.67 3167.16
 3172.85 3175.40 3188.70 3195.67 3199.96 3201.54
 3201.67 3219.27 3223.44 3288.82 3289.43 3291.25
 3312.84 3317.12 3319.43 3619.28 3684.58 3689.13

¹1a-TS (p-NMe₂)

 -335.94 16.95 23.84 29.30 36.04 42.57
 54.35 62.36 66.38 72.63 93.63 97.60
 111.39 136.56 157.72 165.59 170.36 179.42
 182.38 196.84 199.98 210.54 220.96 228.68
 246.54 252.15 269.18 293.78 322.45 342.74
 349.38 351.38 361.01 371.33 375.22 381.20
 406.70 420.49 423.32 425.36 451.61 487.25
 505.13 520.14 522.47 549.73 593.20 603.22
 616.26 634.03 643.66 649.85 650.43 657.26

674.99 689.63 690.54 700.37 703.87 705.07
 720.09 724.99 732.04 735.77 737.76 754.96
 798.11 814.53 815.66 819.08 827.72 828.60
 832.61 841.21 883.31 897.22 934.45 942.23
 943.22 946.15 949.13 951.68 964.36 994.73
 1003.69 1005.02 1009.10 1012.66 1014.71 1017.50
 1024.83 1064.35 1071.89 1086.38 1101.34 1104.56
 1106.19 1107.56 1124.94 1126.22 1132.64 1141.62
 1146.41 1149.80 1156.13 1186.59 1187.93 1200.77
 1201.80 1215.16 1216.58 1221.13 1223.35 1227.35
 1234.43 1241.45 1259.22 1261.85 1274.27 1286.94
 1292.09 1299.20 1320.42 1327.59 1345.59 1364.37
 1368.48 1385.44 1421.01 1421.93 1432.17 1442.02
 1456.05 1458.29 1464.53 1472.76 1473.50 1484.42
 1494.44 1498.22 1501.40 1506.93 1525.92 1538.17
 1540.02 1551.33 1574.98 1599.47 1602.13 1606.03
 1625.16 1648.43 1656.60 2963.63 2974.30 2983.27
 2997.06 3067.05 3069.43 3130.66 3141.29 3167.27
 3175.31 3175.88 3188.20 3193.73 3194.58 3200.67
 3200.90 3218.22 3219.40 3286.86 3288.06 3289.81
 3308.31 3312.32 3314.30 3617.79 3677.26 3687.22

⁵2 (p-NO₂)

 10.68 22.78 26.24 40.45 42.53 54.18
 63.98 65.94 75.17 78.80 85.88 92.90
 109.49 134.35 160.64 164.46 165.25 173.73
 188.45 196.17 213.20 219.41 242.97 246.88
 263.78 267.94 295.35 313.31 317.29 330.17
 334.52 346.33 359.29 370.42 415.33 427.01
 428.18 481.61 509.25 536.85 548.62 596.15
 607.65 614.02 632.47 635.65 646.56 649.47
 651.37 660.43 669.51 695.79 708.38 709.43
 713.67 725.72 729.85 735.72 738.23 750.37
 768.45 771.24 794.84 820.34 839.79 844.68
 853.12 853.96 862.13 867.18 887.06 887.22
 887.61 941.25 942.34 944.56 947.98 955.27
 985.56 995.71 997.57 998.04 1001.37 1003.60
 1006.29 1010.60 1013.34 1030.33 1046.84 1062.23
 1103.03 1104.64 1106.62 1107.75 1108.75 1123.56
 1125.67 1128.96 1130.68 1133.77 1137.14 1188.92
 1192.63 1197.99 1202.54 1207.14 1222.52 1228.53
 1229.83 1239.60 1246.42 1258.92 1278.46 1293.23
 1295.51 1317.72 1319.76 1325.02 1367.44 1370.45
 1392.67 1412.94 1413.24 1415.63 1428.88 1459.48
 1462.28 1463.74 1472.29 1472.69 1526.87 1530.01
 1537.10 1604.20 1606.65 1607.23 1610.89 1624.57
 1648.11 1655.34 1661.46 3007.91 3043.52 3070.08
 3170.20 3177.27 3183.82 3189.78 3194.81 3202.17
 3202.73 3236.22 3240.88 3290.10 3291.82 3292.08
 3319.85 3320.24 3320.50 3645.54 3678.60 3681.56

⁵2 (p-NMe₂)

 15.96 20.78 23.98 40.20 43.85 53.62
 64.88 65.31 76.25 80.06 91.81 98.03
 103.92 114.98 134.00 153.61 163.21 165.58
 167.10 177.43 188.88 195.72 211.76 226.30
 241.87 246.05 248.54 263.36 293.96 301.74
 313.06 321.88 333.26 337.10 346.38 360.56
 397.50 414.95 428.02 433.18 468.33 484.30
 509.72 536.08 575.06 595.05 606.12 617.93
 632.52 646.40 649.37 649.49 660.35 677.62
 686.09 695.28 707.79 712.58 723.36 728.29
 735.10 736.78 749.52 751.02 793.23 794.62
 819.99 831.14 834.45 839.68 841.57 850.92
 869.34 886.12 887.05 940.64 942.07 944.05
 944.75 953.91 956.37 962.69 976.03 996.85
 1000.16 1002.54 1005.45 1010.87 1012.81 1017.03
 1026.96 1051.53 1062.07 1091.37 1102.81 1103.69

1106.07 1107.97 1108.49 1121.95 1127.63 1129.26
1134.54 1135.93 1145.61 1155.47 1183.95 1188.26
1191.75 1202.06 1206.77 1207.94 1222.27 1228.30
1237.26 1238.05 1245.57 1261.03 1261.93 1275.21
1290.63 1297.83 1316.95 1318.32 1340.29 1350.30
1370.11 1399.97 1412.71 1413.79 1415.83 1429.21
1458.06 1458.39 1462.43 1471.05 1472.06 1475.96
1489.39 1501.80 1508.66 1523.28 1524.83 1528.82

1536.80 1566.46 1603.80 1606.05 1609.81 1610.77
1624.45 1655.01 1670.30 2953.90 2997.72 3002.25
3026.04 3040.57 3065.95 3076.01 3120.48 3148.99
3162.15 3168.43 3175.93 3182.12 3188.88 3194.27
3197.96 3201.10 3205.05 3288.49 3288.87 3289.97
3317.06 3318.28 3319.23 3605.19 3678.89 3681.61